

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'HOME' AT 07:10:27 ON 27 JUN 2003  
FILE 'HOME' ENTERED AT 07:10:27 ON 27 JUN 2003

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 1.05             | 1.05          |

=> FIL STNGUIDE

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 1.05             | 1.05          |

FILE 'STNGUIDE' ENTERED AT 07:10:37 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.06             | 1.11          |

FILE 'HOME' ENTERED AT 07:10:40 ON 27 JUN 2003

=> FIL STNGUIDE

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.21             | 1.32          |

FILE 'STNGUIDE' ENTERED AT 07:10:52 ON 27 JUN 2003  
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FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.12             | 1.44          |

FILE 'HOME' ENTERED AT 07:12:21 ON 27 JUN 2003

=> FIL STNGUIDE

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.21             | 1.65          |

FILE 'STNGUIDE' ENTERED AT 07:12:34 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.  
LAST RELOADED: Jun 20, 2003 (20030620/UP).

=> FIL HOME

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY  
0.06

TOTAL  
SESSION  
1.71

FULL ESTIMATED COST

FILE 'HOME' ENTERED AT 07:13:22 ON 27 JUN 2003

=> logoff hold

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY  
0.84

TOTAL  
SESSION  
2.55

FULL ESTIMATED COST

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 07:15:28 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:

LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.  
You either typed them incorrectly, or line noise may  
have corrupted them.

Do you wish to retry the logon?

Enter choice (y/N):

Connecting via Winsock to STN

LOGINID:

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTA1623PAZ

PASSWORD:

LOGINID/PASSWORD REJECTED

The loginid and/or password sent to STN were invalid.  
You either typed them incorrectly, or line noise may  
have corrupted them.

Do you wish to retry the logon?

Enter choice (y/N):

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

|      |    |        |                                                                                               |
|------|----|--------|-----------------------------------------------------------------------------------------------|
| NEWS | 1  |        | Web Page URLs for STN Seminar Schedule - N. America                                           |
| NEWS | 2  |        | "Ask CAS" for self-help around the clock                                                      |
| NEWS | 3  | Jun 03 | New e-mail delivery for search results now available                                          |
| NEWS | 4  | Aug 08 | PHARMAMarketLetter(PHARMAML) - new on STN                                                     |
| NEWS | 5  | Aug 19 | Aquatic Toxicity Information Retrieval (AQUIRE)<br>now available on STN                       |
| NEWS | 6  | Aug 26 | Sequence searching in REGISTRY enhanced                                                       |
| NEWS | 7  | Sep 03 | JAPIO has been reloaded and enhanced                                                          |
| NEWS | 8  | Sep 16 | Experimental properties added to the REGISTRY file                                            |
| NEWS | 9  | Sep 16 | CA Section Thesaurus available in CAPLUS and CA                                               |
| NEWS | 10 | Oct 01 | CASREACT Enriched with Reactions from 1907 to 1985                                            |
| NEWS | 11 | Oct 24 | BEILSTEIN adds new search fields                                                              |
| NEWS | 12 | Oct 24 | Nutraceuticals International (NUTRACEUT) now available on STN                                 |
| NEWS | 13 | Nov 18 | DKILIT has been renamed APOLLIT                                                               |
| NEWS | 14 | Nov 25 | More calculated properties added to REGISTRY                                                  |
| NEWS | 15 | Dec 04 | CSA files on STN                                                                              |
| NEWS | 16 | Dec 17 | PCTFULL now covers WP/PCT Applications from 1978 to date                                      |
| NEWS | 17 | Dec 17 | TOXCENTER enhanced with additional content                                                    |
| NEWS | 18 | Dec 17 | Adis Clinical Trials Insight now available on STN                                             |
| NEWS | 19 | Jan 29 | Simultaneous left and right truncation added to COMPENDEX,<br>ENERGY, INSPEC                  |
| NEWS | 20 | Feb 13 | CANCERLIT is no longer being updated                                                          |
| NEWS | 21 | Feb 24 | METADEX enhancements                                                                          |
| NEWS | 22 | Feb 24 | PCTGEN now available on STN                                                                   |
| NEWS | 23 | Feb 24 | TEMA now available on STN                                                                     |
| NEWS | 24 | Feb 26 | NTIS now allows simultaneous left and right truncation                                        |
| NEWS | 25 | Feb 26 | PCTFULL now contains images                                                                   |
| NEWS | 26 | Mar 04 | SDI PACKAGE for monthly delivery of multifile SDI results                                     |
| NEWS | 27 | Mar 20 | EVENTLINE will be removed from STN                                                            |
| NEWS | 28 | Mar 24 | PATDPAFULL now available on STN                                                               |
| NEWS | 29 | Mar 24 | Additional information for trade-named substances without<br>structures available in REGISTRY |
| NEWS | 30 | Apr 11 | Display formats in DGENE enhanced                                                             |
| NEWS | 31 | Apr 14 | MEDLINE Reload                                                                                |
| NEWS | 32 | Apr 17 | Polymer searching in REGISTRY enhanced                                                        |
| NEWS | 33 | Jun 13 | Indexing from 1947 to 1956 added to records in CA/CAPLUS                                      |
| NEWS | 34 | Apr 21 | New current-awareness alert (SDI) frequency in<br>WPIDS/WPINDEX/WPIX                          |
| NEWS | 35 | Apr 28 | RDISCLOSURE now available on STN                                                              |
| NEWS | 36 | May 05 | Pharmacokinetic information and systematic chemical names<br>added to PHAR                    |
| NEWS | 37 | May 15 | MEDLINE file segment of TOXCENTER reloaded                                                    |
| NEWS | 38 | May 15 | Supporter information for ENCOMPAT and ENCOMPLIT updated                                      |
| NEWS | 39 | May 16 | CHEMREACT will be removed from STN                                                            |
| NEWS | 40 | May 19 | Simultaneous left and right truncation added to WSCA                                          |
| NEWS | 41 | May 19 | RAPRA enhanced with new search field, simultaneous left and<br>right truncation               |
| NEWS | 42 | Jun 06 | Simultaneous left and right truncation added to CBNB                                          |
| NEWS | 43 | Jun 06 | PASCAL enhanced with additional data                                                          |
| NEWS | 44 | Jun 20 | 2003 edition of the FSTA Thesaurus is now available                                           |
| NEWS | 45 | Jun 25 | HSDB has been reloaded                                                                        |

NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
 MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
 AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003-  
 NEWS HOURS STN Operating Hours Plus Help Desk Availability  
 NEWS INTER General Internet Information  
 NEWS LOGIN Welcome Banner and News Items  
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
 NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
 specific topic.

All use of STN is subject to the provisions of the STN Customer  
 agreement. Please note that this agreement limits use to scientific  
 research. Use for software development or design or implementation  
 of commercial gateways or other similar uses is prohibited and may  
 result in loss of user privileges and other penalties.

\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 08:29:25 ON 27 JUN 2003

=> logoff hold

|                      |            |         |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL   |
|                      | ENTRY      | SESSION |
| FULL ESTIMATED COST  | 0.84       | 0.84    |

SESSION WILL BE HELD FOR 60 MINUTES  
 STN INTERNATIONAL SESSION SUSPENDED AT 08:31:42 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
 SESSION RESUMED IN FILE 'HOME' AT 08:44:40 ON 27 JUN 2003  
 FILE 'HOME' ENTERED AT 08:44:40 ON 27 JUN 2003

|                      |            |         |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL   |
|                      | ENTRY      | SESSION |
| FULL ESTIMATED COST  | 0.84       | 0.84    |

=> file mreg

'MREG' IS NOT A VALID FILE NAME  
 SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files  
 that are available. If you have requested multiple files, you can  
 specify a corrected file name or you can enter "IGNORE" to continue  
 accessing the remaining file names entered.

=> file reg

|                      |            |         |
|----------------------|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL   |
|                      | ENTRY      | SESSION |
| FULL ESTIMATED COST  | 1.05       | 1.05    |

FILE 'REGISTRY' ENTERED AT 08:45:01 ON 27 JUN 2003  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8  
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP  
PROPERTIES for more information. See STN Note 27, Searching Properties  
in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 10075845 generic six.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search l1 sss sam

SAMPLE SEARCH INITIATED 08:45:37 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS

3 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 58448 TO 65112

PROJECTED ANSWERS: 3 TO 367

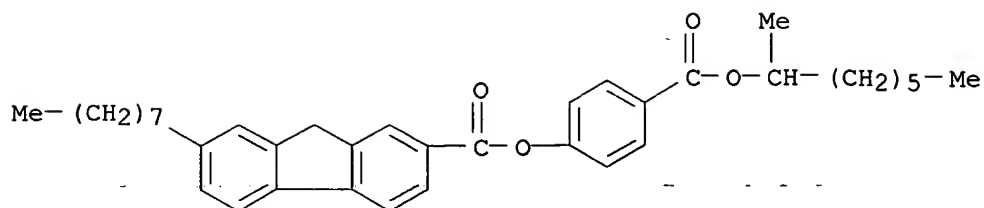
L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[[[1-  
methylheptyl]oxy]carbonyl]phenyl ester (9CI)

MF C37 H46 O4



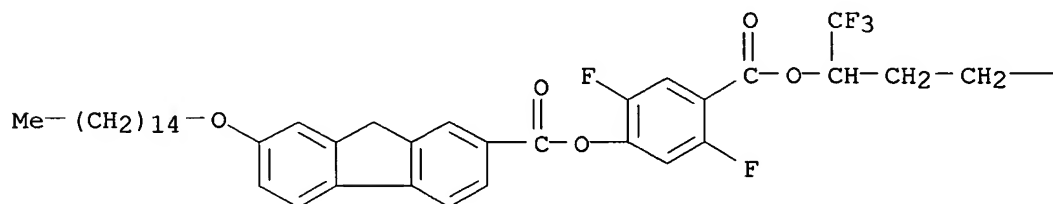
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):lofgoff hold  
'LOFGOFF HOLD' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".  
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN 9H-Fluorene-2-carboxylic acid, 7-(pentadecyloxy)-, 4-[[[4-ethyl-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2,5-difluorophenyl ester (9CI)  
MF C45 H57 F5 O5

PAGE 1-A

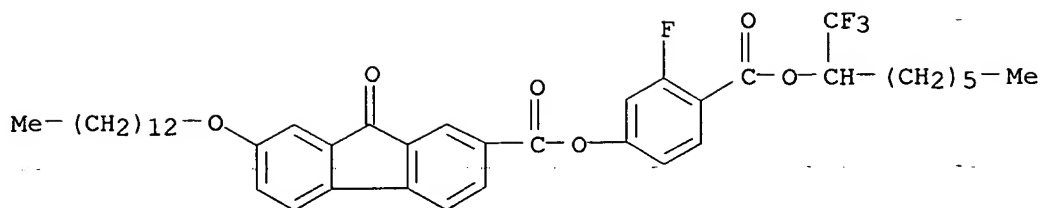


PAGE 1-B

— CHEt<sub>2</sub>

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN 9H-Fluorene-2-carboxylic acid, 9-oxo-7-(tridecyloxy)-, 3-fluoro-4-[[[1-(trifluoromethyl)heptyl]oxy]carbonyl]phenyl ester (9CI)  
MF C42 H50 F4 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 0.80       | 1.85    |

FULL ESTIMATED COST

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 08:46:27 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*

SESSION RESUMED IN FILE 'REGISTRY' AT 08:48:38 ON 27 JUN 2003

FILE 'REGISTRY' ENTERED AT 08:48:38 ON 27 JUN 2003

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COST IN U.S. DOLLARS

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 0.80       | 1.85    |

FULL ESTIMATED COST

=>

Uploading 10075845 generic six.str

L3 STRUCTURE UPLOADED

=> d 113

L13 NOT FOUND

The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> d 13

L3 HAS NO ANSWERS

L3 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search l3 sss sam  
 SAMPLE SEARCH INITIATED 08:49:58 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS 0 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 58448 TO 65112  
 PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=> search l3 sss full  
 FULL SEARCH INITIATED 08:50:14 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 62195 TO ITERATE

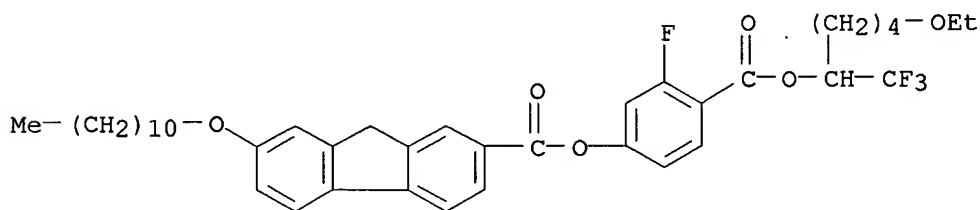
100.0% PROCESSED 62195 ITERATIONS 137 ANSWERS  
 SEARCH TIME: 00.00.03

L5 137 SEA SSS FUL L3

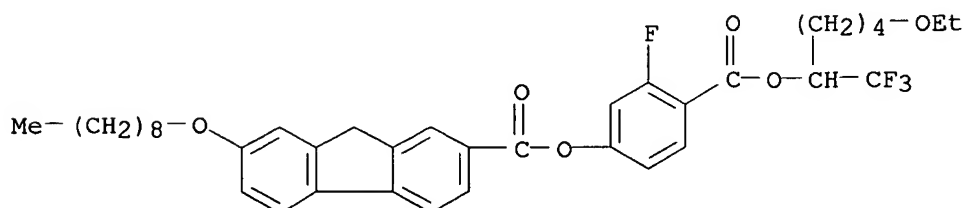
=> d scan

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with  
 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl  
 7-(undecyloxy)-9H-fluorene-2-carboxylate, 1-methylheptyl  
 4-[6-(4-hexylphenyl)-3-pyridinyl]benzoate, 4-[[1-(1-methylheptyl)oxy]carbonyl]phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate and 4-[[1-(1-methylheptyl)oxy]carbonyl]phenyl  
 4-[[4-(undecyloxy)benzoyl]oxy]benzoate (9CI)  
 MF C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C32 H41 N O2  
 CI MXS

CM 1

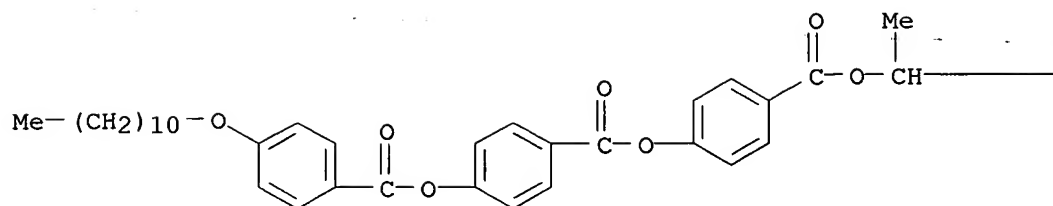


CM 2



CM 3

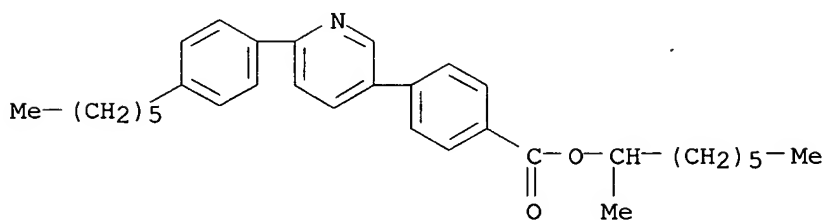
PAGE 1-A



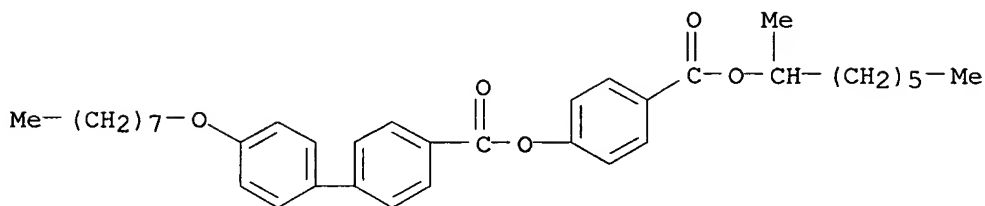
PAGE 1-B

— (CH<sub>2</sub>)<sub>5</sub>—Me

CM 4



CM 5

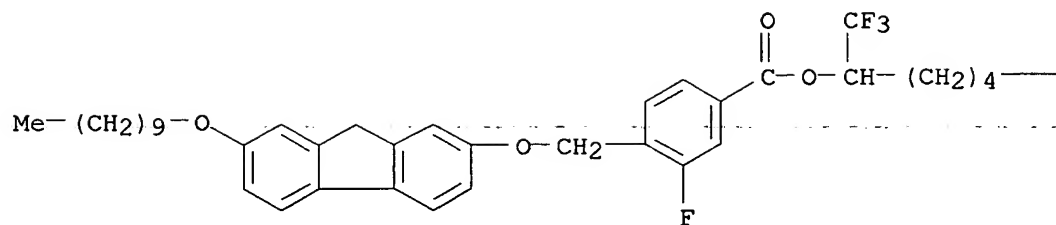


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):20

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 4-[[[7-(decyloxy)-9H-fluoren-2-yl]oxy]methyl]-3-fluoro-,  
5-ethoxy-1-(trifluoromethyl)pentyl ester (9CI)

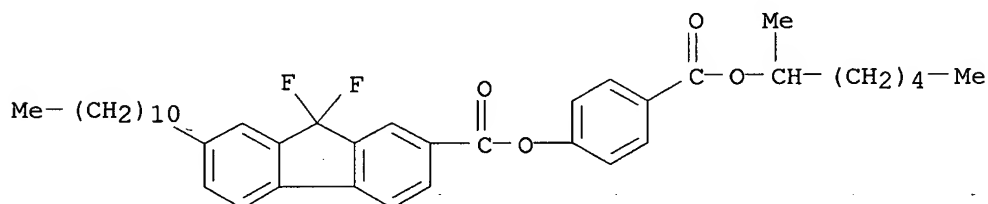
MF C39 H48 F4 O5



—OEt

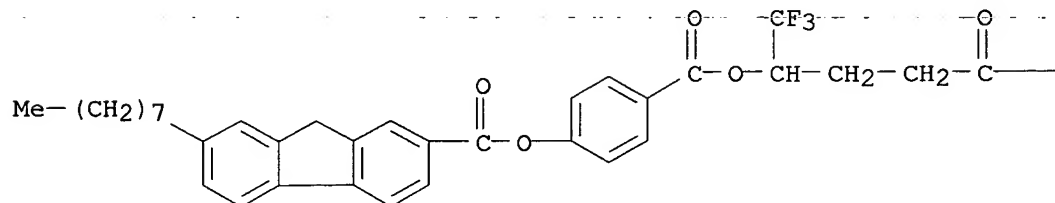
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 9,9-difluoro-7-undecyl-,  
 4-[[[1-methylhexyl]oxy]carbonyl]phenyl ester (9CI)  
 MF C39 H48 F2 O4



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-octyl-, 4-[[[4-butoxy-4-oxo-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)  
 MF C38 H43 F3 O6

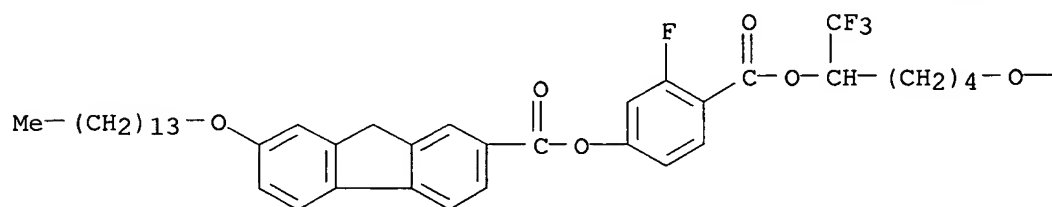


— OBU-n

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 3-fluoro-4-[[2,2,2-trifluoro-1-[4-(2,2,2-trifluoroethoxy)butyl]ethoxy]carbonyl]phenyl ester (9CI)  
 MF C43 H51 F7 O6

PAGE 1-A

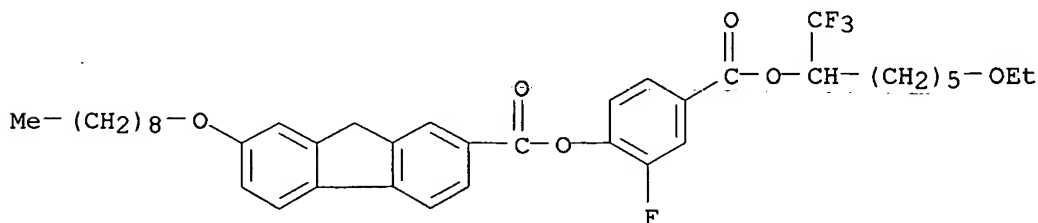


PAGE 1-B

— CH<sub>2</sub>— CF<sub>3</sub>

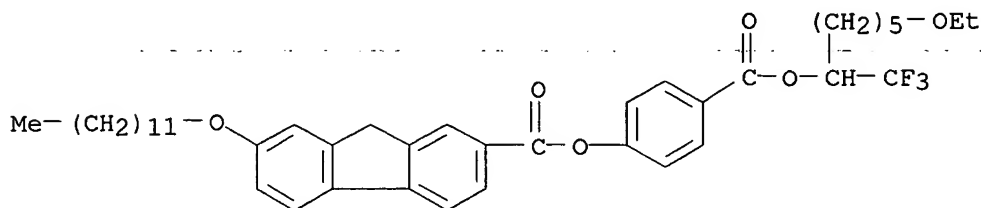
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]-2-fluorophenyl ester (9CI)  
 MF C39 H46 F4 O6



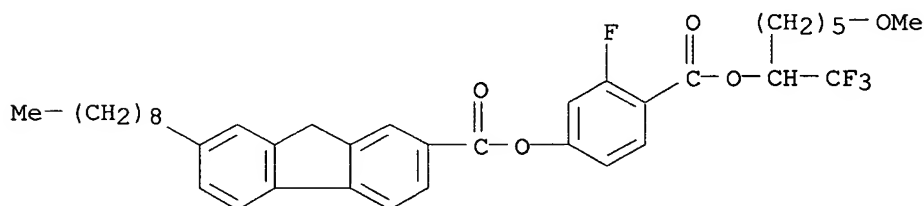
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[[6-ethoxy-1-(trifluoromethyl)hexyl]oxy]carbonyl]phenyl ester (9CI)  
 MF C42 H53 F3 O6



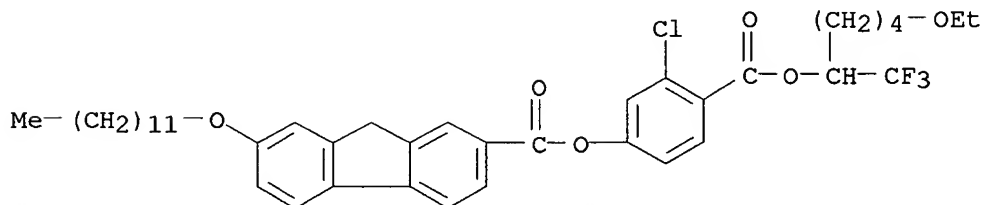
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-nonyl-, 3-fluoro-4-[[[2,2,2-trifluoro-1-(5-methoxypentyl)ethoxy]carbonyl]phenyl ester (9CI)  
 MF C38 H44 F4 O5



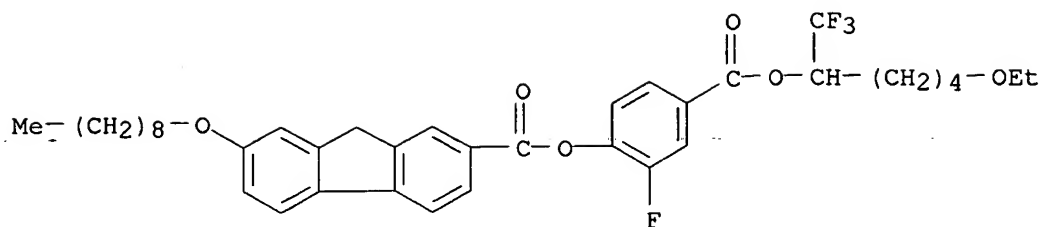
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 3-chloro-4-[[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]phenyl ester (9CI)  
 MF C41 H50 Cl F3 O6



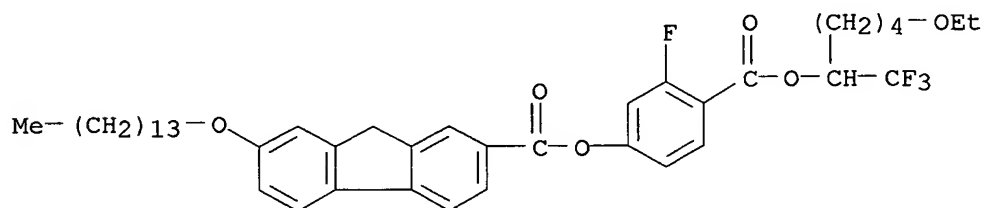
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-2-fluorophenyl ester (9CI)  
 MF C38 H44 F4 O6



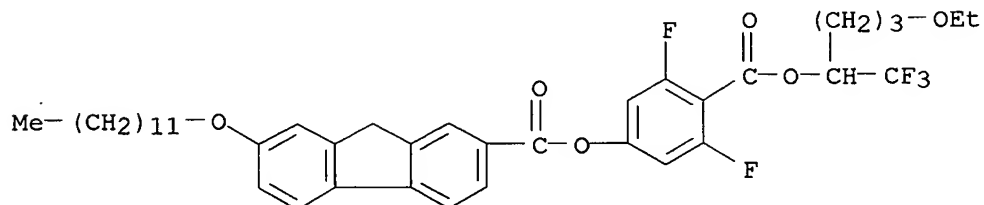
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(tetradecyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester (9CI)  
 MF C43 H54 F4 O6



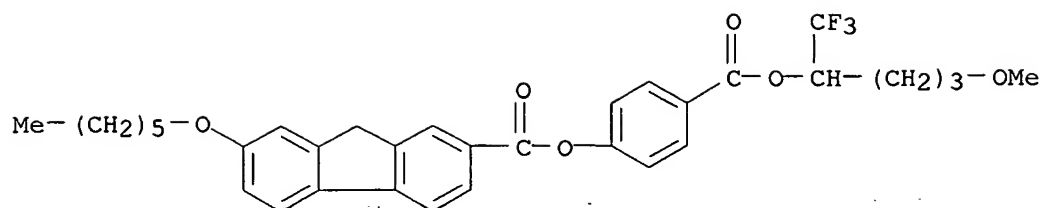
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[4-ethoxy-1-(trifluoromethyl)butoxy]carbonyl]-3,5-difluorophenyl ester (9CI)  
 MF C40 H47 F5 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

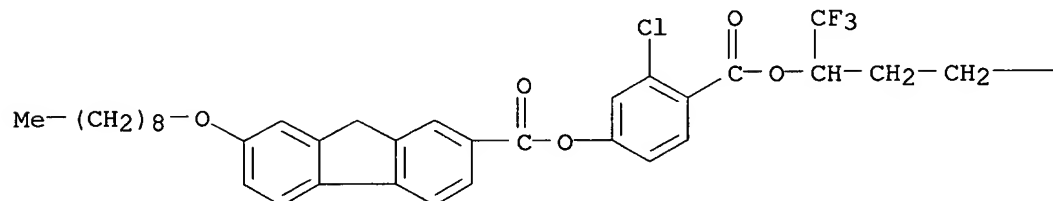
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[[4-methoxy-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)  
 MF C33 H35 F3 O6



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 3-chloro-4-[[3-ethoxy-1-(trifluoromethyl)propoxy]carbonyl]phenyl ester (9CI)  
 MF C36 H40 Cl F3 O6

PAGE 1-A

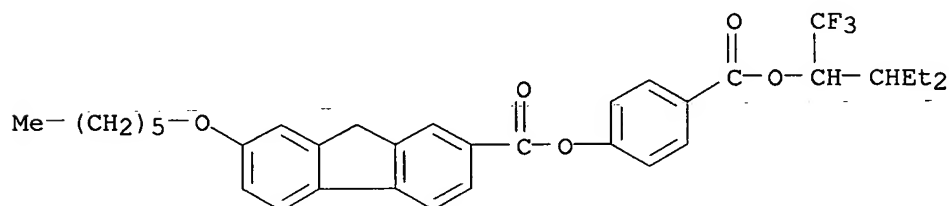


PAGE 1-B

—OEt

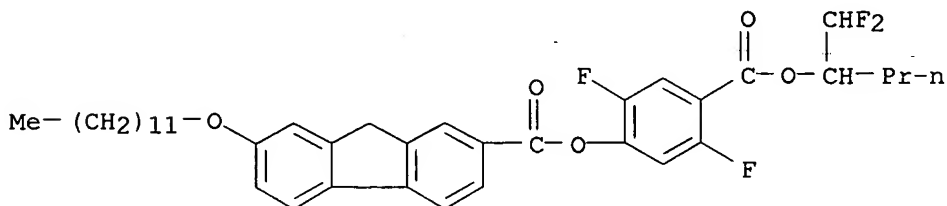
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(hexyloxy)-, 4-[[2-ethyl-1-(trifluoromethyl)butoxy]carbonyl]phenyl ester (9CI)  
 MF C34 H37 F3 O5



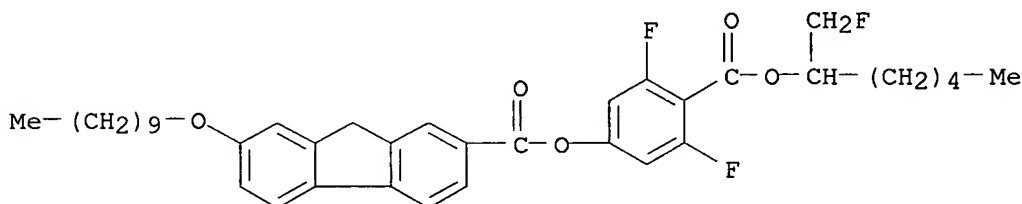
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(dodecyloxy)-, 4-[[1-(difluoromethyl)butoxy]carbonyl]-2,5-difluorophenyl ester (9CI)  
 MF C38 H44 F4 O5



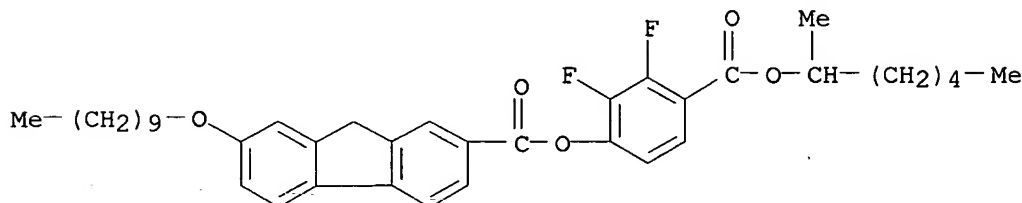
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 3,5-difluoro-4-[[[1-(fluoromethyl)hexyl]oxy]carbonyl]phenyl ester (9CI)  
 MF C38 H45 F3 O5



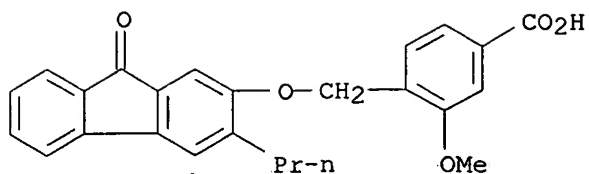
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(decyloxy)-, 2,3-difluoro-4-[[[1-methylhexyl]oxy]carbonyl]phenyl ester (9CI)  
 MF C38 H46 F2 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 3-methoxy-4-[[[9-oxo-3-propyl-9H-fluoren-2-yl]oxy]methyl]- (9CI)  
 MF C25 H22 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

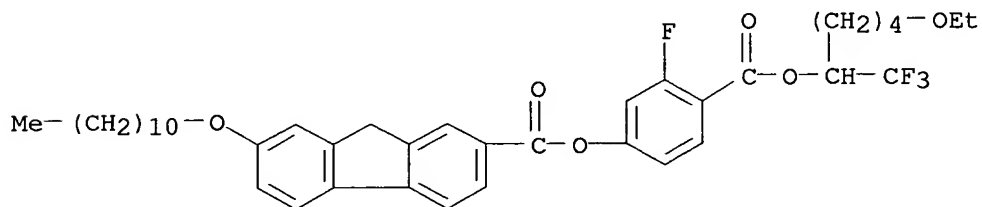
L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN 9H-Fluorene-2-carboxylic acid, 7-(nonyloxy)-, 4-[[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with 4-[[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl 7-(undecyloxy)-9H-fluorene-2-carboxylate, 4-[[[1-methylheptyl]oxy]carbonyl]phenyl 4-(octyloxy)benzoate, 4-[[[1-methylheptyl]oxy]carbonyl]phenyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate and 4-[[[1-methylheptyl]oxy]carbonyl]phenyl 4-[[4-(undecyloxy)benzoyl]oxy]benzoate (9CI)

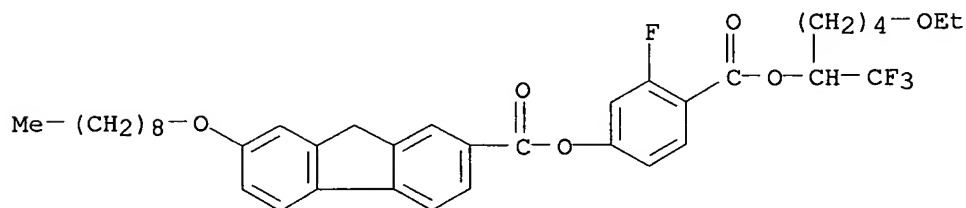
MF C40 H52 O7 . C40 H48 F4 O6 . C38 H44 F4 O6 . C36 H46 O5 . C30 H42 O5

CI MXS

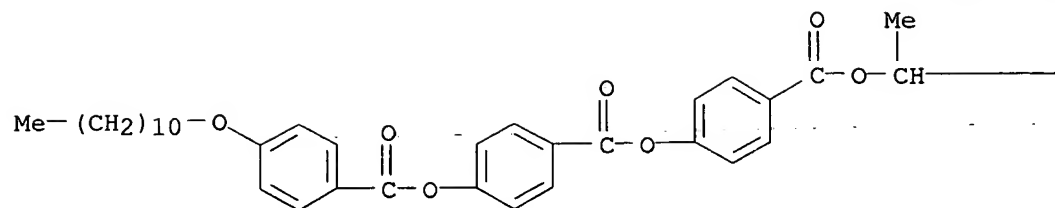
CM 1



CM 2

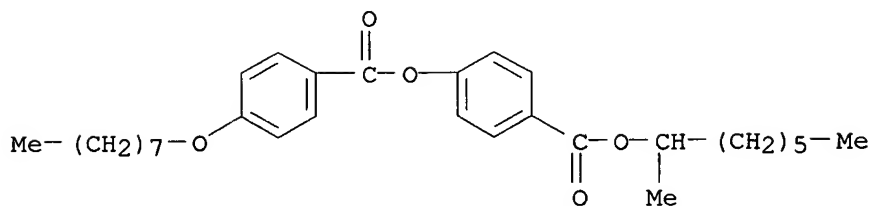


CM 3

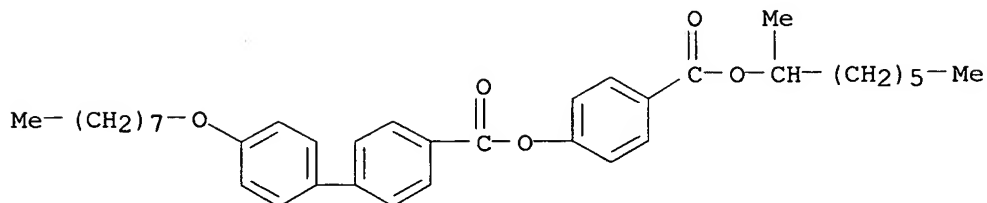


— (CH<sub>2</sub>)<sub>5</sub>—Me

CM 4

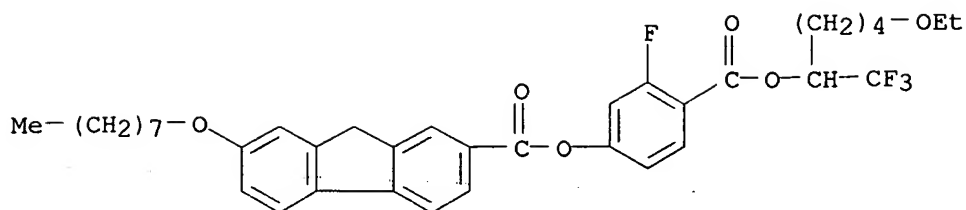


CM 5

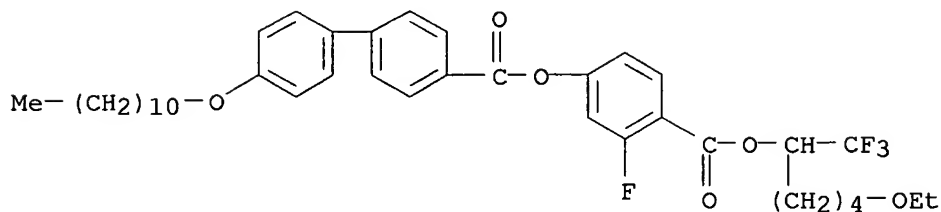


L5 137 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN 9H-Fluorene-2-carboxylic acid, 7-(octyloxy)-, 4-[[1-(4-ethoxybutyl)-2,2,2-trifluoroethoxy]carbonyl]-3-fluorophenyl ester, mixt. with  
 4-[[[5-ethoxy-1-(trifluoromethyl)pentyl]oxy]carbonyl]-3-fluorophenyl  
 4'-(undecyloxy)[1,1'-biphenyl]-4-carboxylate (9CI)  
 MF C39 H48 F4 O6 . C37 H42 F4 O6  
 CI MXS

CM 1



CM 2



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>

Uploading 10075845 generic six.str

L6 STRUCTURE UPLOADED

=> d l6

L6 HAS NO ANSWERS

L6 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search l6 sss sam

SAMPLE SEARCH INITIATED 08:54:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 58448 TO 65112

PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> search l6 sss full

FULL SEARCH INITIATED 08:54:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 62195 TO ITERATE

100.0% PROCESSED 62195 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.03

L8

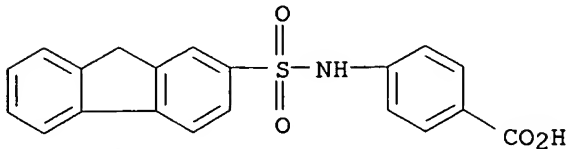
3 SEA SSS FUL L6

=> d scan

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 4-[(9H-fluoren-2-ylsulfonyl)amino]- (9CI)

MF C20 H15 N O4 S



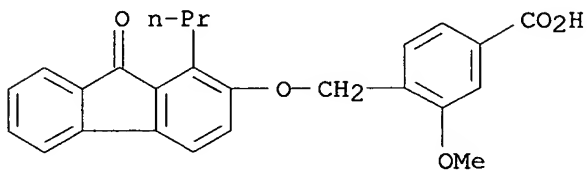
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 3-methoxy-4-[[ (9-oxo-1-propyl-9H-fluoren-2-yl)oxy]methyl]- (9CI)

MF C25 H22 O5

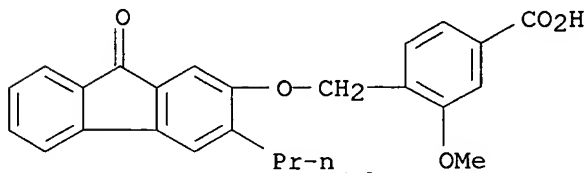


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 3 ANSWERS REGISTRY COPYRIGHT 2003 ACS

IN Benzoic acid, 3-methoxy-4-[[ (9-oxo-3-propyl-9H-fluoren-2-yl)oxy]methyl]- (9CI)

MF C25 H22 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 301.90           | 302.95        |

SESSION WILL BE HELD FOR 60 MINUTES  
STN INTERNATIONAL SESSION SUSPENDED AT 08:57:09 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

\* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \*  
SESSION RESUMED IN FILE 'REGISTRY' AT 09:05:09 ON 27 JUN 2003  
FILE 'REGISTRY' ENTERED AT 09:05:09 ON 27 JUN 2003  
COPYRIGHT (C) 2003 American Chemical Society (ACS)

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 301.90           | 302.95        |

=>

Uploading 10075845 generic six crrct.str

L9 STRUCTURE UPLOADED

=> d 19

L9 HAS NO ANSWERS

L9 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search 19 sss sam

SAMPLE SEARCH INITIATED 09:06:14 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 3229 TO ITERATE

|                                           |                 |           |
|-------------------------------------------|-----------------|-----------|
| 31.0% PROCESSED                           | 1000 ITERATIONS | 0 ANSWERS |
| INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) |                 |           |
| SEARCH TIME: 00.00.01                     |                 |           |

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 61173 TO 67987  
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM\_L9

=> search 19 sss full

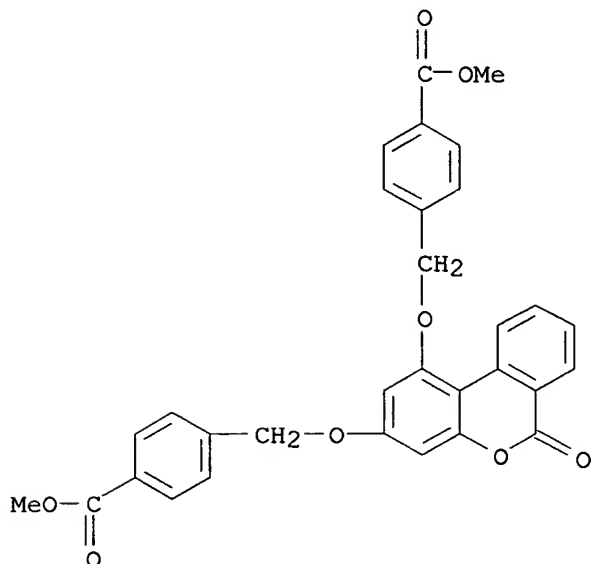
FULL SEARCH INITIATED 09:06:24 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 65007 TO ITERATE

|                       |                  |           |
|-----------------------|------------------|-----------|
| 100.0% PROCESSED      | 65007 ITERATIONS | 6 ANSWERS |
| SEARCH TIME: 00.00.03 |                  |           |

L11 6 SEA SSS FUL L9

=> d scan

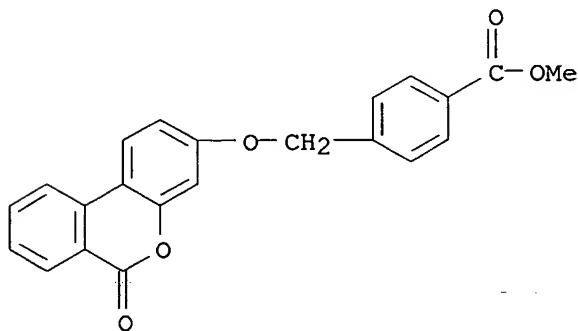
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4,4'-[(6-oxo-6H-dibenzo[b,d]pyran-1,3-diyl)bis(oxymethylene)]bis-, dimethyl ester (9CI)  
MF C31 H24 O8



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):6

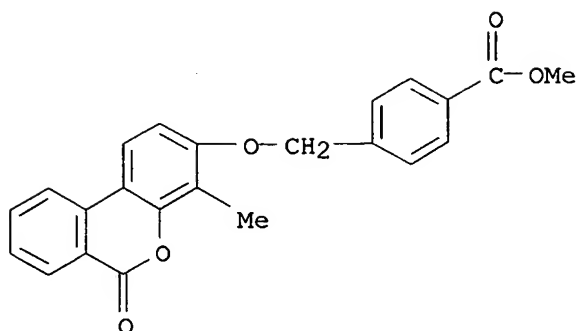
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[[(6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester (9CI)  
MF C22 H16 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

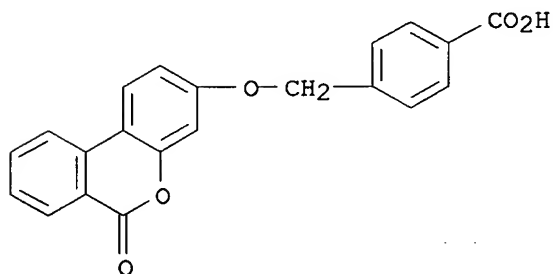
L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[[(4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-,

methyl ester (9CI)  
MF C23 H18 O5



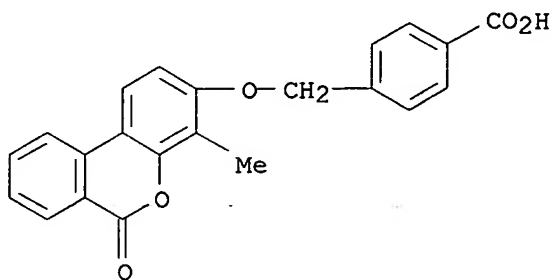
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[ (6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]- (9CI)  
MF C21 H14 O5



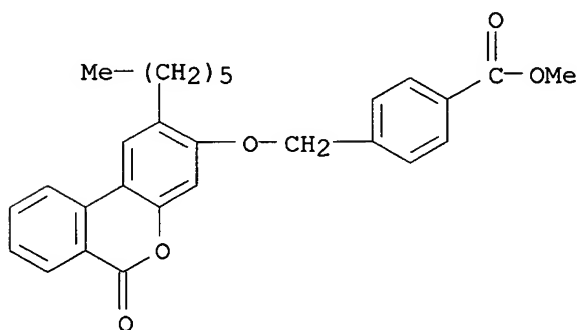
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
IN Benzoic acid, 4-[[ (4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-  
(9CI)  
MF C22 H16 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L11 6 ANSWERS REGISTRY COPYRIGHT 2003 ACS  
 IN Benzoic acid, 4-[[ (2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-,  
 methyl ester (9CI)  
 MF C28 H28 O5



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

COST IN U.S. DOLLARS

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 452.05     | 453.10  |

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 09:09:01 ON 27 JUN 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26  
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 16

**REGISTRY INITIATED**

Substance data SEARCH and crossover from CAS REGISTRY in progress...  
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:09:05 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 3089 TO ITERATE

32.4% PROCESSED 1000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 58448 TO 65112  
PROJECTED ANSWERS: 0 TO 0

L12 0 SEA SSS SAM L6

L13 0 L12

=> 111

L14 0 L11

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.42             | 454.34        |

FILE 'CAPLUS' ENTERED AT 09:09:41 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26

FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l11

L15 0 L11

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 0.42             | 454.76        |

FILE 'REGISTRY' ENTERED AT 09:10:33 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8  
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STN Note 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> search l9 sss full

FULL SEARCH INITIATED 09:10:50 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 65007 TO ITERATE

100.0% PROCESSED 65007 ITERATIONS 6 ANSWERS  
SEARCH TIME: 00.00.03

L16 6 SEA SSS FUL L9

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST  | 148.15           | 602.91        |

FILE 'CAPLUS' ENTERED AT 09:11:00 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
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FILE COVERS 1907 - 27 Jun 2003 VOL 138 ISS 26  
FILE LAST UPDATED: 25 Jun 2003 (20030625/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> l16

L17 0 L16

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.42

603.33

FILE 'REGISTRY' ENTERED AT 09:11:36 ON 27 JUN 2003  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8  
DICTIONARY FILE UPDATES: 25 JUN 2003 HIGHEST RN 537653-06-8

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> e Benzoic acid, 4-(((6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy)methyl)-/cn  
E1 1 BENZOIC ACID, 4-(((6-O-ACETYL-2,3,4-TRIS-O-(PHENYLMETHYL)-.A  
LPHA.-D-MANNOPYRANOSYL)OXY)METHYL)-3-NITRO-, METHYL ESTER/CN  
E2 1 BENZOIC ACID, 4-(((6-OXO-2,4-CYCLOHEXADIEN-1-YLIDENE)METHYL)  
AMINO)-, METHYL ESTER/CN  
E3 0 --> BENZOIC ACID, 4-(((6-OXO-6H-DIBENZOB,DPYRAN-3-YL)OXY)METHY  
L)-/CN  
E4 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHY  
L)-/CN  
E5 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO(B,D)PYRAN-3-YL)OXY)METHY  
L)-, METHYL ESTER/CN  
E6 1 BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO)THIOXOMETHYL)AMINO)-,  
METHYL ESTER/CN  
E7 1 BENZOIC ACID, 4-(((6R)-6-(((2S)-2-(ACETYLAMINO)-1-OXO-3-(4-(  
PHOSPHONOOXY)PHENYL)PROPYL)AMINO)TETRAHYDRO-5-OXO-1,4-THIAZE  
PIN-4(5H)-YL)METHYL)-, 1-METHYL ESTER/CN  
E8 1 BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL)THIO)-/CN  
E9 1 BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)  
BENZOYL)AMINO)-1,4-THIAZEPIN-4(5H)-YL)METHYL)-, 1-METHYL EST  
ER/CN  
E10 1 BENZOIC ACID, 4-(((6R,12AR)-6-(1,3-BENZODIOXOL-5-YL)-3,4,6,7

, 12, 12A-HEXAHYDRO-1, 4-DIOXOPYRAZINO (1', 2': 1, 6) PYRIDO (3, 4-B) I  
NDOL-2 (1H) -YL) METHYL) -/CN

E11 1 BENZOIC ACID, 4-(((6R, 12AR)-6-(1, 3-BENZODIOXOL-5-YL)-3, 4, 6, 7  
, 12, 12A-HEXAHYDRO-1, 4-DIOXOPYRAZINO (1', 2': 1, 6) PYRIDO (3, 4-B) I  
NDOL-2 (1H) -YL) METHYL) -, METHYL ESTER/CN

E12 1 BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL) METHYL)  
-2-METHYL-4, 7-DIOXO-1-(((PHENYLMETHYL) AMINO) CARBONYL) -8H-PYR  
AZINO (2, 1-C) (1, 2, 4) TRIAZIN-8-YL) METHYL) -/CN

=> e Benzoic acid, 4-(((6-oxo-6H-dibenzo (b, d) pyran-3-yl) oxy) methyl) -/cn

E1 1 BENZOIC ACID, 4-(((6-O-ACETYL-2, 3, 4-TRIS-O- (PHENYLMETHYL) -.A  
LPHA.-D-MANNOPYRANOSYL) OXY) METHYL) -3-NITRO-, METHYL ESTER/CN

E2 1 BENZOIC ACID, 4-(((6-OXO-2, 4-CYCLOHEXADIEN-1-YLIDENE) METHYL)  
AMINO) -, METHYL ESTER/CN

E3 1 --> BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO (B, D) PYRAN-3-YL) OXY) METHY  
L) -/CN

E4 1 BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO (B, D) PYRAN-3-YL) OXY) METHY  
L) -, METHYL ESTER/CN

E5 1 BENZOIC ACID, 4-(((6-QUINOXALINYLAMINO) THIOXOMETHYL) AMINO) -,  
METHYL ESTER/CN

E6 1 BENZOIC ACID, 4-(((6R)-6-(((2S)-2-(ACETYLAMINO) -1-OXO-3-(4-(  
PHOSPHONOOXY) PHENYL) PROPYL) AMINO) TETRAHYDRO-5-OXO-1, 4-THIAZE  
PIN-4 (5H) -YL) METHYL) -, 1-METHYL ESTER/CN

E7 1 BENZOIC ACID, 4-(((6R)-7-CARBOXY-6-HYDROXYHEPTYL) THIO) -/CN

E8 1 BENZOIC ACID, 4-(((6R)-TETRAHYDRO-5-OXO-6-((4-(PHOSPHONOOXY)  
BENZOYL) AMINO) -1, 4-THIAZEPIN-4 (5H) -YL) METHYL) -, 1-METHYL EST  
ER/CN

E9 1 BENZOIC ACID, 4-(((6R, 12AR)-6-(1, 3-BENZODIOXOL-5-YL)-3, 4, 6, 7  
, 12, 12A-HEXAHYDRO-1, 4-DIOXOPYRAZINO (1', 2': 1, 6) PYRIDO (3, 4-B) I  
NDOL-2 (1H) -YL) METHYL) -/CN

E10 1 BENZOIC ACID, 4-(((6R, 12AR)-6-(1, 3-BENZODIOXOL-5-YL)-3, 4, 6, 7  
, 12, 12A-HEXAHYDRO-1, 4-DIOXOPYRAZINO (1', 2': 1, 6) PYRIDO (3, 4-B) I  
NDOL-2 (1H) -YL) METHYL) -, METHYL ESTER/CN

E11 1 BENZOIC ACID, 4-(((6S)-OCTAHYDRO-6-((4-HYDROXYPHENYL) METHYL)  
-2-METHYL-4, 7-DIOXO-1-(((PHENYLMETHYL) AMINO) CARBONYL) -8H-PYR  
AZINO (2, 1-C) (1, 2, 4) TRIAZIN-8-YL) METHYL) -/CN

E12 1 BENZOIC ACID, 4-(((6S, 9.ALPHA., 11.ALPHA., 13E, 15S)-6, 9-EPOXY-  
11, 15-DIHYDROXY-1-OXOPROSTA-7, 13-DIEN-1-YL) AMINO) -/CN

=> e3

L18 1 "BENZOIC ACID, 4-(((6-OXO-6H-DIBENZO (B, D) PYRAN-3-YL) OXY) METHYL) -  
"/CN

=> d 118

L18 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

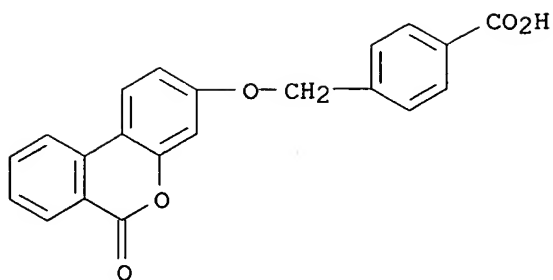
RN 314744-77-9 REGISTRY

CN Benzoic acid, 4-[[ (6-oxo-6H-dibenzo [b, d] pyran-3-yl) oxy] methyl] -  
(9CI) (CA INDEX NAME)

MF C21 H14 O5

SR Chemical Library

LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

=> file chemcats

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

7.10

610.43

FILE 'CHEMCATS' ENTERED AT 09:13:31 ON 27 JUN 2003

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=> l16

L19 22 L16

=> d 11911-22 ti

'L1911-22' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

'TI' IS NOT A VALID FORMAT FOR FILE 'CHEMCATS'

The following are valid formats:

The default display format is IDE.

ALL ---- AN, CO, PD, ON, CN, RN, ST, Purity, Impurity, product identifiers, product notes, STR, product text (properties, regulatory information, references, prices, warnings, miscellaneous fields), CO, CA, CY, TX (products, terms, and conditions; products and services;

packaging and snipping; safety and handling; other  
supplier information)

COMP --- AN, CO, PD, CO, TX  
 IDE ---- AN, CO, PD, ON, CN, RN, LSF, ST, STR  
 MISC --- AN, miscellaneous product information fields  
 PINFO -- AN, pricing information text  
 PRICE -- AN, prices, quantities  
 PROD --- AN, product text  
 PROP --- AN, properties  
 REF ---- AN, references  
 REGS --- AN, regulatory information  
 SAFE --- AN, product warnings  
 SINFO -- AN, safety text  
 HIT ---- All fields containing hit terms  
 KWIC --- All hit terms plus 20 words on either side  
 OCC ---- List of display fields containing hit terms

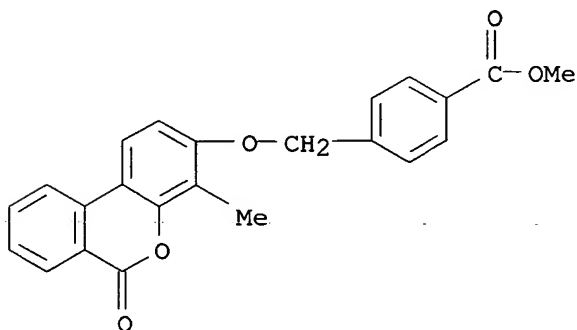
Hit terms will be highlighted in all displayable fields.

To display a particular field or fields, enter the display field codes. For a list of display field codes, enter 'HELP DFIELDS' at an arrow prompt (=>). Examples include: 'KWIC'; 'CN RN'; 'IDE CO'. You may specify the formats and fields in any order, and the information will be displayed in the same order as the format specification.

The same formats (except for HIT, KWIC, and OCC) may be used with the DISPLAY ACC command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (IDE):ide

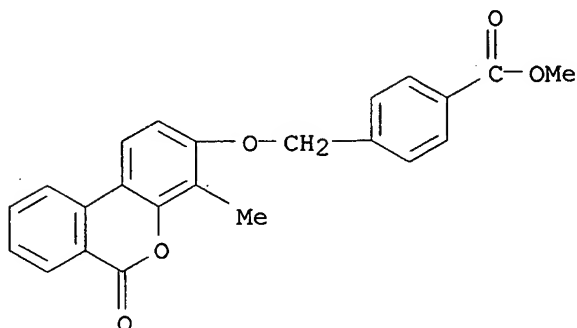
L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2003:2193953 CHEMCATS  
 Catalog Name (CO): ChemDiv, Inc. Product Library  
 Publication Date (PD): 25 Apr 2003  
 Order Number (ON): 3330-4466  
 Chemical Name (CN): Benzoic acid, 4-[[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-62-8**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



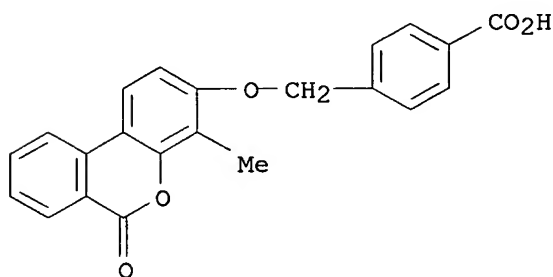
=> d l19 1-22 ide

L19 ANSWER 1 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2003:2193953 CHEMCATS  
 Catalog Name (CO): ChemDiv, Inc. Product Library  
 Publication Date (PD): 25 Apr 2003  
 Order Number (ON): 3330-4466  
 Chemical Name (CN): Benzoic acid, 4-[[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): 307551-62-8  
 Supplementary Term (ST): CHEMICAL LIBRARY  
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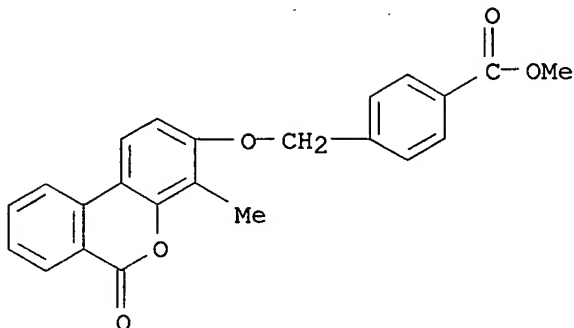


L19 ANSWER 2 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2003:884552 CHEMCATS  
 Catalog Name (CO): Ambinter: Exploratory Library  
 Publication Date (PD): 30 Apr 2003  
 Order Number (ON): 7210430945  
 Chemical Name (CN): Benzoic acid, 4-[[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-  
 CAS Registry No. (RN): 314744-95-1  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

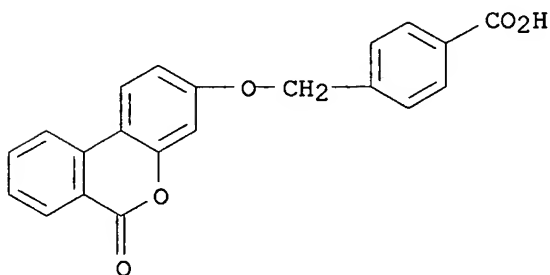


L19 ANSWER 3 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2003:884551 CHEMCATS  
 Catalog Name (CO): Ambinter: Exploratory Library  
 Publication Date (PD): 30 Apr 2003  
 Order Number (ON): 7210430944  
 Chemical Name (CN): Benzoic acid, 4-[[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 Synonym (CN): Also sold under Ambinter order number(s) F0398-0417, t0310-3431  
 CAS Registry No. (RN): 307551-62-8

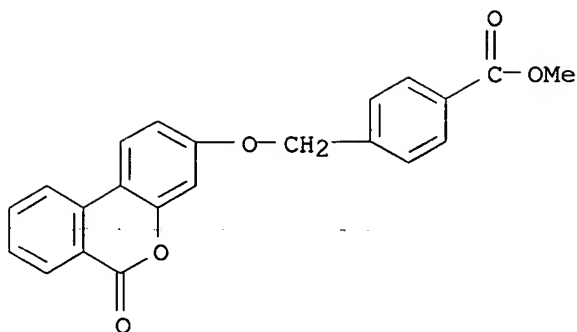
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



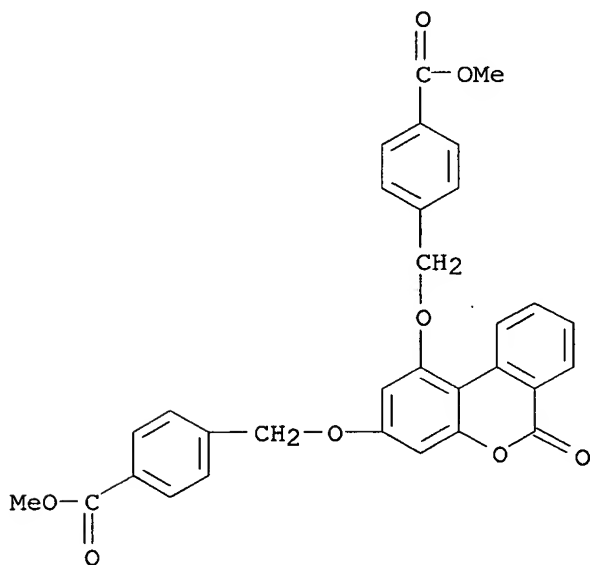
L19 ANSWER 4 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2003:884511 CHEMCATS  
Catalog Name (CO): Ambinter: Exploratory Library  
Publication Date (PD): 30 Apr 2003  
Order Number (ON): 7210430903  
Chemical Name (CN): Benzoic acid, 4-[[ (6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-  
CAS Registry No. (RN): **314744-77-9**  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



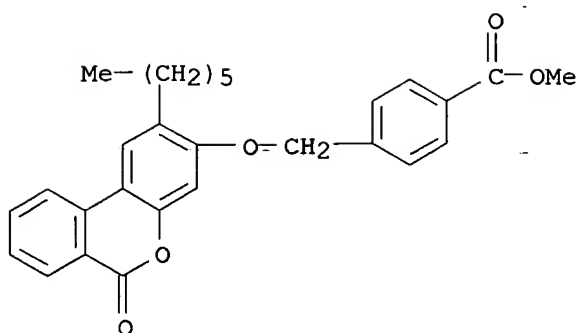
L19 ANSWER 5 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
Accession No. (AN): 2003:884510 CHEMCATS  
Catalog Name (CO): Ambinter: Exploratory Library  
Publication Date (PD): 30 Apr 2003  
Order Number (ON): 7210430902  
Chemical Name (CN): Benzoic acid, 4-[[ (6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
Synonym (CN): Also sold under Ambinter order number(s) F0398-0388  
CAS Registry No. (RN): **307551-40-2**  
Supplementary Term (ST): CHEMICAL LIBRARY  
Structure :



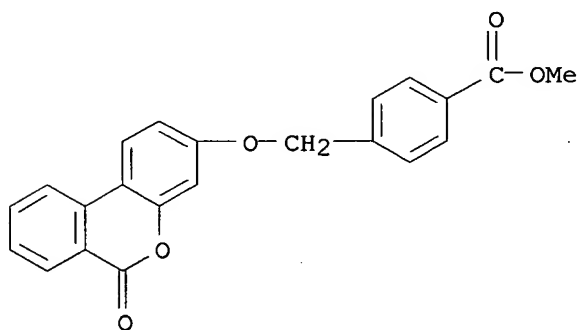
L19 ANSWER 6 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2833186 CHEMCATS  
 Catalog Name (CO): Ambinter: Exploratory Library  
 Publication Date (PD): 30 Apr 2003  
 Order Number (ON): t0304-3777  
 Chemical Name (CN): Benzoic acid, 4,4'-[(6-oxo-6H-dibenzo[b,d]pyran-1,3-diyl)bis(oxymethylene)]bis-, dimethyl ester  
 CAS Registry No. (RN): **438035-34-8**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



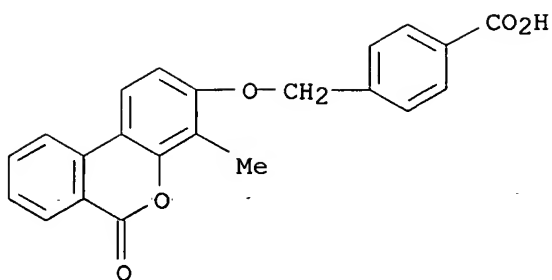
L19 ANSWER 7 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2800180 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2002  
 Order Number (ON): 7212010324  
 Chemical Name (CN): Benzoic acid, 4-[[[(2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **405917-31-9**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



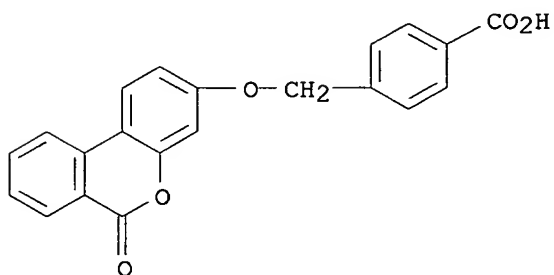
L19 ANSWER 8 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2796908 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2002  
 Order Number (ON): 7210430902  
 Chemical Name (CN): Benzoic acid, 4-[[ (6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-40-2**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



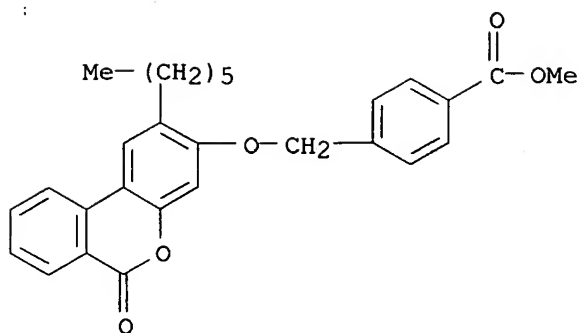
L19 ANSWER 9 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2768171 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2002  
 Order Number (ON): 7210430945  
 Chemical Name (CN): Benzoic acid, 4-[[ (4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-  
 CAS Registry No. (RN): **314744-95-1**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L19 ANSWER 10 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2768153 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2002  
 Order Number (ON): 7210430903  
 Chemical Name (CN): Benzoic acid, 4-[[ (6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-  
 CAS Registry No. (RN): **314744-77-9**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

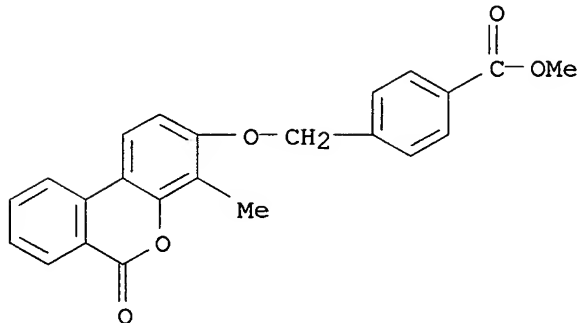


L19 ANSWER 11 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2002:2276618 CHEMCATS  
 Catalog Name (CO): Ambinter: Exploratory Library  
 Publication Date (PD): 30 Apr 2003  
 Order Number (ON): 7212010324  
 Chemical Name (CN): Benzoic acid, 4-[[ (2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl)oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **405917-31-9**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



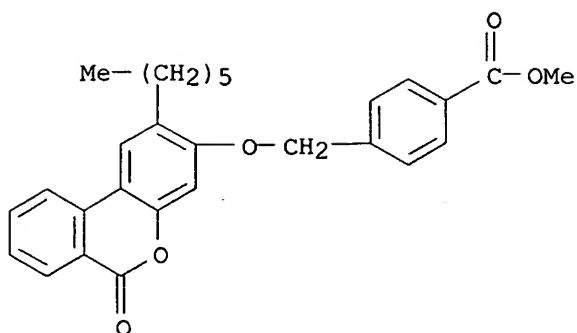
L19 ANSWER 12 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:2147072 CHEMCATS  
 Catalog Name (CO): Interchim Intermediates  
 Publication Date (PD): 9 Jul 2002  
 Order Number (ON): 3330-4466  
 Chemical Name (CN): Benzoic acid, 4-[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl-, methyl ester  
 Synonym (CN): Also sold under Interchim order number(s) 7210430944, F0398-0417  
 CAS Registry No. (RN): **307551-62-8**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



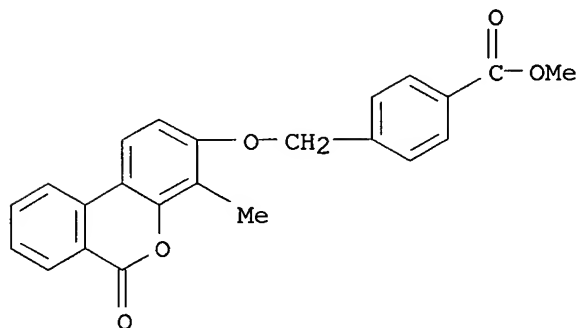
L19 ANSWER 13 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:1324350 CHEMCATS  
 Catalog Name (CO): Otava Stock Chemicals  
 Publication Date (PD): 28 May 2003  
 Order Number (ON): 7212010324  
 Chemical Name (CN): Benzoic acid, 4-[[2-hexyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl-, methyl ester  
 CAS Registry No. (RN): **405917-31-9**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



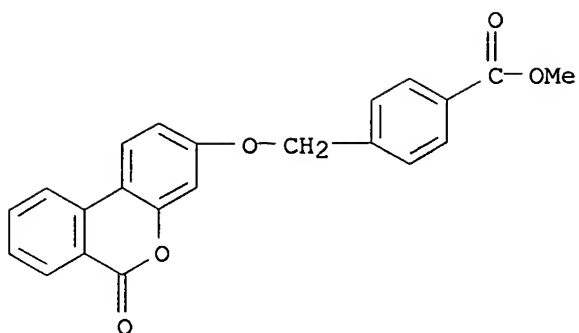
L19 ANSWER 14 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2002:607872 CHEMCATS  
 Catalog Name (CO): ChemBridge Product List  
 Publication Date (PD): 17 Jan 2002  
 Order Number (ON): 6166000  
 Chemical Name (CN): Benzoic acid, 4-[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-62-8**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
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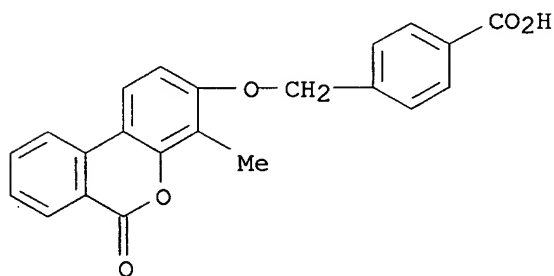


L19 ANSWER 15 OF 22 CHEMCATS COPYRIGHT 2003 ACS

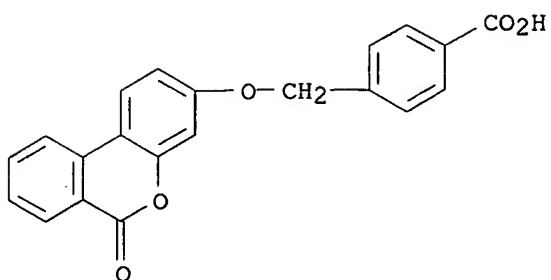
Accession No. (AN): 2002:605953 CHEMCATS  
 Catalog Name (CO): ChemBridge Product List  
 Publication Date (PD): 17 Jan 2002  
 Order Number (ON): 6145952  
 Chemical Name (CN): Benzoic acid, 4-[[6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-40-2**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



L19 ANSWER 16 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2001:131979 CHEMCATS  
 Catalog Name (CO): Otava Chemical Collection  
 Publication Date (PD): 21 Apr 2003  
 Order Number (ON): 7210430945  
 Chemical Name (CN): Benzoic acid, 4-[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-  
 CAS Registry No. (RN): **314744-95-1**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :

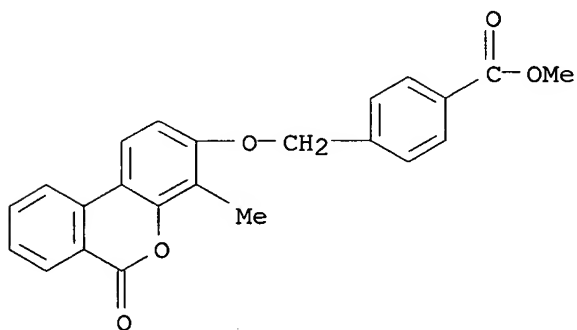


L19 ANSWER 17 OF 22 CHEMCATS COPYRIGHT 2003 ACS  
 Accession No. (AN): 2001:131961 CHEMCATS  
 Catalog Name (CO): Otava Chemical Collection  
 Publication Date (PD): 21 Apr 2003  
 Order Number (ON): 7210430903  
 Chemical Name (CN): Benzoic acid, 4-[[6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-  
 CAS Registry No. (RN): **314744-77-9**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



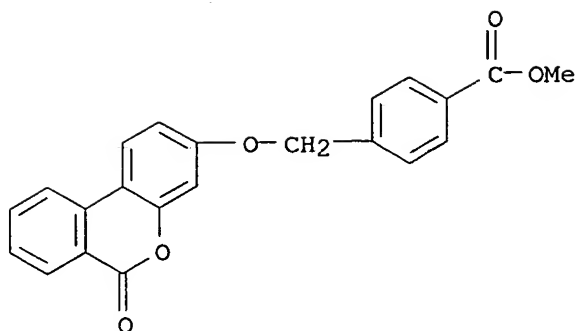
L19 ANSWER 18 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:1065757 CHEMCATS  
 Catalog Name (CO): Otava Stock Chemicals  
 Publication Date (PD): 28 May 2003  
 Order Number (ON): 7210430944  
 Chemical Name (CN): Benzoic acid, 4-[[4-methyl-6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-62-8**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
 Structure :



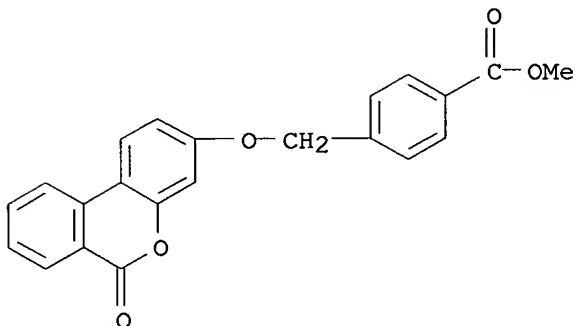
L19 ANSWER 19 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:1065735 CHEMCATS  
 Catalog Name (CO): Otava Stock Chemicals  
 Publication Date (PD): 28 May 2003  
 Order Number (ON): 7210430902  
 Chemical Name (CN): Benzoic acid, 4-[[6-oxo-6H-dibenzo[b,d]pyran-3-yl]oxy]methyl]-, methyl ester  
 CAS Registry No. (RN): **307551-40-2**  
 Supplementary Term (ST): CHEMICAL LIBRARY  
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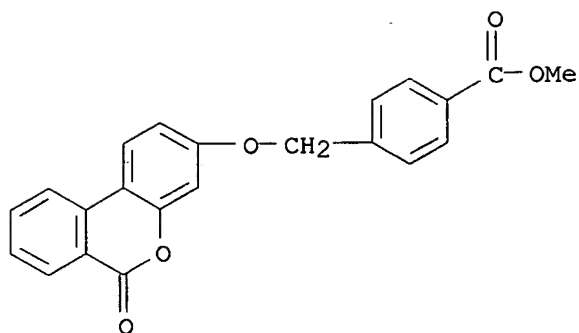
L19 ANSWER 20 OF 22 CHEMCATS COPYRIGHT 2003 ACS

|                    |                                                                        |          |
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| Accession No.      | (AN): 2000:899357                                                      | CHEMCATS |
| Catalog Name       | (CO): SALOR                                                            |          |
| Publication Date   | (PD): 15 Jan 2003                                                      |          |
| Order Number       | (ON): R632457                                                          |          |
| Chemical Name      | (CN): METHYL 4-((6-OXO-6H-BENZO(C) CHROMEN-3-YL) OXY) METHYL) BENZOATE |          |
| CAS Registry No.   | (RN): 307551-40-2                                                      |          |
| Supplementary Term | (ST): CHEMICAL LIBRARY                                                 |          |
| Structure          | :                                                                      |          |



L19 ANSWER 21 OF 22 CHEMCATS COPYRIGHT 2003 ACS

|                    |                                                                        |          |
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| Accession No.      | (AN): 2000:897302                                                      | CHEMCATS |
| Catalog Name       | (CO): SALOR                                                            |          |
| Publication Date   | (PD): 15 Jan 2003                                                      |          |
| Order Number       | (ON): R609854                                                          |          |
| Chemical Name      | (CN): METHYL 4-((6-OXO-6H-BENZO(C) CHROMEN-3-YL) OXY) METHYL) BENZOATE |          |
| CAS Registry No.   | (RN): 307551-40-2                                                      |          |
| Supplementary Term | (ST): CHEMICAL LIBRARY                                                 |          |
| Structure          | :                                                                      |          |



L19 ANSWER 22 OF 22 CHEMCATS COPYRIGHT 2003 ACS

Accession No. (AN): 2000:434091 CHEMCATS

Catalog Name (CO): SALOR

Publication Date (PD): 15 Jan 2003

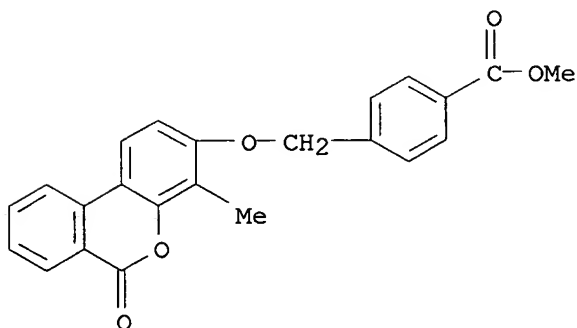
Order Number (ON): R503738

Chemical Name (CN): 4-(4-METHYL-6-OXO-6H-BENZO(C)CHROMEN-3-YLOXYMETHYL)-  
BENZOIC ACID METHYL ESTER

CAS Registry No. (RN): 307551-62-8

Supplementary Term (ST): CHEMICAL LIBRARY

Structure :



=> logoff hold

COST IN U.S. DOLLARS

FULL ESTIMATED COST

| SINCE FILE | TOTAL   |
|------------|---------|
| ENTRY      | SESSION |
| 43.20      | 653.63  |

SESSION WILL BE HELD FOR 60 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 09:16:46 ON 27 JUN 2003

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

|      |         |        |                                                                                                                                                           |
|------|---------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|
| NEWS | 1       |        | Web Page URLs for STN Seminar Schedule - N. America                                                                                                       |
| NEWS | 2       |        | "Ask CAS" for self-help around the clock                                                                                                                  |
| NEWS | 3       | Jun 03 | New e-mail delivery for search results now available                                                                                                      |
| NEWS | 4       | Aug 08 | PHARMAMarketLetter(PHARMAML) - new on STN                                                                                                                 |
| NEWS | 5       | Aug 19 | Aquatic Toxicity Information Retrieval (AQUIRE)<br>now available on STN                                                                                   |
| NEWS | 6       | Aug 26 | Sequence searching in REGISTRY enhanced                                                                                                                   |
| NEWS | 7       | Sep 03 | JAPIO has been reloaded and enhanced                                                                                                                      |
| NEWS | 8       | Sep 16 | Experimental properties added to the REGISTRY file                                                                                                        |
| NEWS | 9       | Sep 16 | CA Section Thesaurus available in CAPLUS and CA                                                                                                           |
| NEWS | 10      | Oct 01 | CASREACT Enriched with Reactions from 1907 to 1985                                                                                                        |
| NEWS | 11      | Oct 24 | BEILSTEIN adds new search fields                                                                                                                          |
| NEWS | 12      | Oct 24 | Nutraceuticals International (NUTRACEUT) now available on STN                                                                                             |
| NEWS | 13      | Nov 18 | DKILIT has been renamed APOLLIT                                                                                                                           |
| NEWS | 14      | Nov 25 | More calculated properties added to REGISTRY                                                                                                              |
| NEWS | 15      | Dec 04 | CSA files on STN                                                                                                                                          |
| NEWS | 16      | Dec 17 | PCTFULL now covers WP/PCT Applications from 1978 to date                                                                                                  |
| NEWS | 17      | Dec 17 | TOXCENTER enhanced with additional content                                                                                                                |
| NEWS | 18      | Dec 17 | Adis Clinical Trials Insight now available on STN                                                                                                         |
| NEWS | 19      | Jan 29 | Simultaneous left and right truncation added to COMPENDEX,<br>ENERGY, INSPEC                                                                              |
| NEWS | 20      | Feb 13 | CANCERLIT is no longer being updated                                                                                                                      |
| NEWS | 21      | Feb 24 | METADEX enhancements                                                                                                                                      |
| NEWS | 22      | Feb 24 | PCTGEN now available on STN                                                                                                                               |
| NEWS | 23      | Feb 24 | TEMA now available on STN                                                                                                                                 |
| NEWS | 24      | Feb 26 | NTIS now allows simultaneous left and right truncation                                                                                                    |
| NEWS | 25      | Feb 26 | PCTFULL now contains images                                                                                                                               |
| NEWS | 26      | Mar 04 | SDI PACKAGE for monthly delivery of multifile SDI results                                                                                                 |
| NEWS | 27      | Mar 20 | EVENTLINE will be removed from STN                                                                                                                        |
| NEWS | 28      | Mar 24 | PATDPAFULL now available on STN                                                                                                                           |
| NEWS | 29      | Mar 24 | Additional information for trade-named substances without<br>structures available in REGISTRY                                                             |
| NEWS | 30      | Apr 11 | Display formats in DGENE enhanced                                                                                                                         |
| NEWS | 31      | Apr 14 | MEDLINE Reload                                                                                                                                            |
| NEWS | 32      | Apr 17 | Polymer searching in REGISTRY enhanced                                                                                                                    |
| NEWS | 33      | Jun 13 | Indexing from 1947 to 1956 added to records in CA/CAPLUS                                                                                                  |
| NEWS | 34      | Apr 21 | New current-awareness alert (SDI) frequency in<br>WPIDS/WPINDEX/WPIX                                                                                      |
| NEWS | 35      | Apr 28 | RDISCLOSURE now available on STN                                                                                                                          |
| NEWS | 36      | May 05 | Pharmacokinetic information and systematic chemical names<br>added to PHAR                                                                                |
| NEWS | 37      | May 15 | MEDLINE file segment of TOXCENTER reloaded                                                                                                                |
| NEWS | 38      | May 15 | Supporter information for ENCOMPAT and ENCOMPLIT updated                                                                                                  |
| NEWS | 39      | May 16 | CHEMREACT will be removed from STN                                                                                                                        |
| NEWS | 40      | May 19 | Simultaneous left and right truncation added to WSCA                                                                                                      |
| NEWS | 41      | May 19 | RAPRA enhanced with new search field, simultaneous left and<br>right truncation                                                                           |
| NEWS | 42      | Jun 06 | Simultaneous left and right truncation added to CBNB                                                                                                      |
| NEWS | 43      | Jun 06 | PASCAL enhanced with additional data                                                                                                                      |
| NEWS | 44      | Jun 20 | 2003 edition of the FSTA Thesaurus is now available                                                                                                       |
| NEWS | 45      | Jun 25 | HSDB has been reloaded                                                                                                                                    |
| NEWS | EXPRESS |        | April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT<br>MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),<br>AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003 |
| NEWS | HOURS   |        | STN Operating Hours Plus Help Desk Availability                                                                                                           |
| NEWS | INTER   |        | General Internet Information                                                                                                                              |

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NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

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FILE COVERS 1907 - 7 Jul 2003 VOL 139 ISS 2

FILE LAST UPDATED: 6 Jul 2003 (20030706/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> arotinoids

L1 54 AROTINOIDS

=> retinobenzoic

L2 40 RETINO BENZOIC

=> l1 and l2

L3 0 L1 AND L2

=> phenan?

L4 62851 PHENAN?

=> l1 and l4

L5 0 L1 AND L4

=> d l1 44-54 ti

L1 ANSWER 44 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI The effects of **arotinoids** on rat mammary carcinogenesis

L1 ANSWER 45 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Retinoid-induced changes of lipid synthesis in cultured human epidermal keratinocytes

L1 ANSWER 46 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Diazacholesterol-induced ichthyosis in the hairless mouse

L1 ANSWER 47 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Sulfur-containing **arotinoids**, a new class of retinoids

L1 ANSWER 48 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Synergistic effect of retinoic acid on DNA synthesis by prostaglandin F2.alpha. stimulated Swiss 3T3 cells

L1 ANSWER 49 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Effects of **arotinoids** upon murine embryonal carcinoma cells

L1 ANSWER 50 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Retinoic acid enhances the initiation of DNA synthesis stimulated by prostaglandin F2.alpha. in Swiss 3T3 cells

L1 ANSWER 51 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Affinity therapeutics. 1. Selective incorporation of 2-thiouracil derivatives in murine melanomas. Cytostatic activity of 2-thiouracil **arotinoids**, 2-thiouracil retinoids, **arotinoids**, and retinoids

L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI Structure-activity relationship of retinoids in fetal rat bone cultures

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**, a new class of highly active retinoids

=> d 11 52-54 ti fbib abs

L1 ANSWER 52 OF 54 CAPLUS COPYRIGHT 2003 ACS

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

AN 1982:141529 CAPLUS

DN 96:141529

TI **Arotinoids**. A new class of retinoids with activities in oncology and dermatology

AU Bollag, Werner

CS Pharma Res. Dep., F. Hoffmann-La Roche und Co. Ltd., Basel, Switz.

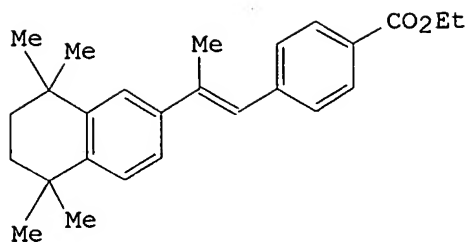
SO Cancer Chemotherapy and Pharmacology (1981), 7(1), 27-9

CODEN: CCPHDZ; ISSN: 0344-5704

DT Journal

LA English

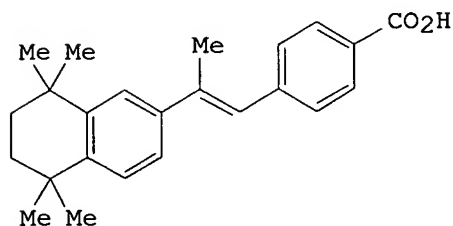
GI



I

AB **Arotinoids** are a new class of retinoids with particular biol. properties. Arotinoid Ro 13-6298 (I) [71441-09-3] in minute quantities leads to regression of chem. induced papillomas of the skin of mice. The ratio between the antipapilloma effect and the toxic syndrome of hypervitaminosis A is very favorable. Ro 13-6298 also has a therapeutic influence on chem. induced skin carcinomas in mice. As the papilloma model has proved to be suitable for screening for antipsoriatic and antikeratinizing properties as well as for antineoplastic screening, arotinoids might be useful in human clin. dermatol. and oncol.

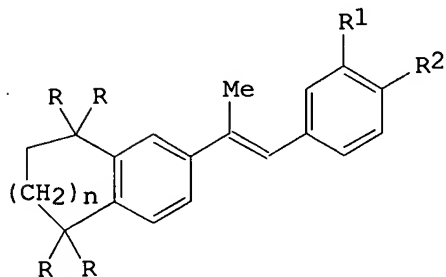
L1 ANSWER 53 OF 54 CAPLUS COPYRIGHT 2003 ACS  
 TI Structure-activity relationship of retinoids in fetal rat bone cultures  
 AN 1981:525879 CAPLUS  
 DN 95:125879  
 TI Structure-activity relationship of retinoids in fetal rat bone cultures  
 AU Kistler, Andreas  
 CS Biol. Pharm. Res. Dep., F. Hoffmann-La Roche Co. Ltd., Basel, CH-4002, Switz.  
 SO Calcified Tissue International (1981), 33(3), 249-54  
 CODEN: CTINDZ; ISSN: 0171-967X  
 DT Journal  
 LA English  
 GI



I

AB The structure-activity relation of 29 retinoids was investigated in fetal rat bone organ cultures. Retinoids induced the release of proteoglycan followed by cartilage tissue breakdown. The loss of RNA was used as a parameter for cartilage resorption. During 6 days of incubation, RNA decreased up to 80% in the presence of active retinoids. The ED40 was detd. from dose-response curves of the various retinoids. The new compds., called **arotinoids**, which contained the retinoic acid C skeleton in a fixed cisoid geometric conformation, were up to 200 times more active than all-trans-.beta.-retinoic acid. The most active compd. was I [71441-28-6]. Several lines of evidence indicated that the carboxylic acid end group was essential for the activity of retinoids in fetal bone cultures. These new, highly active retinoids might be an excellent tool to investigate whether the retinoid action is mediated by specific cellular retinoid binding proteins.

L1 ANSWER 54 OF 54 CAPLUS COPYRIGHT 2003 ACS  
 TI **Arotinoids**, a new class of highly active retinoids  
 AN 1980:586020 CAPLUS  
 DN 93:186020  
 TI **Arotinoids**, a new class of highly active retinoids  
 AU Loeliger, Peter; Bollag, Werner; Mayer, Hans  
 CS F. Hoffmann-La Roche and Co. Ltd., Basel, CH 4002, Switz.  
 SO European Journal of Medicinal Chemistry (1980), 15(1), 9-15  
 CODEN: EJMCA5; ISSN: 0009-4374  
 DT Journal  
 LA English  
 GI



I

AB A new class of retinoids, named **arotinoids** (I), R = H or Me, R1 = H, R2 = COEt, n = 0; R = R1 = Me, R2 = CO2Et, n = 1; R = Me, R1 = H, R2 = H, Me, CHO, CH2OH, CH2OMe, CH2OAc, CO2H, CO2Et, CO2CHMe2, CO2CMe3 or CONHET, n = 1), which had up to 10 times more favorable therapeutic ratio for papilloma regression than retinoic acid (II) were prepd. by the Wittig reaction of (1-arylethyl)triphenylphosphonium bromides with benzaldehydes. E.g., Me 5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl ketone was reduced, the alc. converted to the bromide, and this was quaternized with Ph3P and reacted with 4-HCOC6H4CO2Et to give (E)-I (R = Me, R1 = H, R2 = CO2Et, n = 1), which had therapeutic potency in the antipapilloma test 8000 times that of II while the toxic hypervitaminosis A effects were increased by 800 times.

=> tricyc?

L6 30539 TRICYC?

=> d his

(FILE 'HOME' ENTERED AT 13:10:23 ON 07 JUL 2003)

FILE 'CAPLUS' ENTERED AT 13:10:30 ON 07 JUL 2003

L1 54 AROTINOIDS  
 L2 40 RETINO BENZOIC  
 L3 0 L1 AND L2  
 L4 62851 PHENAN?  
 L5 0 L1 AND L4  
 L6 30539 TRICYC?

=> l1 and l6

L7 0 L1 AND L6

=> ?arotinoids

L8 298 ?AROTINOIDS

=> carotinoids

L9 209 CAROTINOIDS

=> 18 not 19

L10 89 L8 NOT L9

=> 110 not 11

L11 35 L10 NOT L1

=> benzo?

L12 475881 BENZO?

=> 111 and 112

L13 15 L11 AND L12

=> d 113 1-15 ti

L13 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties

L13 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions

L13 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

L13 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic cultures of ovarian carcinoma

L13 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis, Structure-Activity Relationships, and RAR. $\gamma$ -Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]

L13 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic acid**-11-[14C]

L13 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis, Structure-Activity Relationships, and RAR. $\gamma$ -Ligand Interactions of Nitrogen **Heteroarotinoids**

L13 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI synthesis, receptor specificity and TGase activity of **heteroarotinoids**-anticancer-agents-

L13 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

L13 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI **Heteroarotinoids**: crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl]**benzoate**

L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Novel **heteroarotinoids**: synthesis and biological activity

L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI **Heteroarotinoids**: analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Heteroarotinoid compounds as anticancer agents

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**

=> benzoarotinoid?

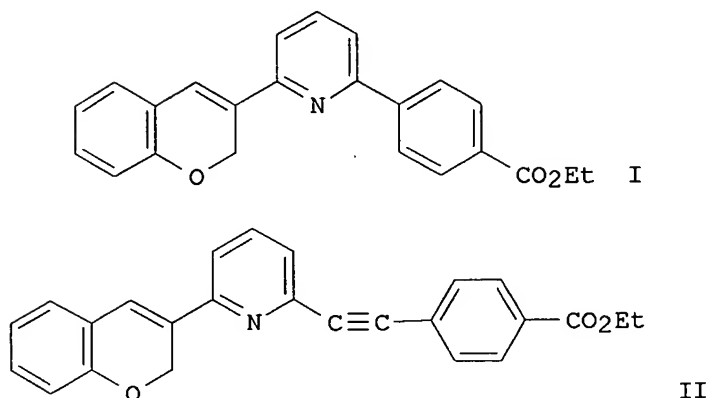
L14 0 BENZOAROTINOID?

=> d l13 1-15 ti fbib abs

L13 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties  
 AN 2003:322782 CAPLUS  
 TI Novel Chiral, Sulfur-Containing **Heteroarotinoids** with Liquid Crystal Properties  
 AU Weerasekare, G. Mahika; Berlin, K. Darrell; Sunkara, Haribabu; Ford, Warren T.  
 CS Oklahoma State University, Stillwater, OK, USA  
 SO Phosphorus, Sulfur and Silicon and the Related Elements (2003), 178(5), 993-1006  
 CODEN: PSSLEC; ISSN: 1042-6507  
 PB Taylor & Francis Ltd.  
 DT Journal  
 LA English  
 AB Synthetic methods were developed to prep. Et (E)-4-[2-(3,4-dihydro-2-n-octyl-1-oxy-2H-1-**benzothio**-pyran-6-yl)-1-propenyl]**benzoate** (1) and Et (E)-4-[2-(3,4-dihydro-2-n-octyl-2H-1-**benzothiopyran**-6-yl)-1-propenyl]**benzoate** (10). These are the first examples of **heteroarotinoids** which possess properties of liq. crystals. The properties were evaluated using differential scanning calorimetry and by use of polarizing microg. Both displayed textures which are typical of a smectic or cholesteric phase.

L13 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions  
 AN 2001:867362 CAPLUS  
 DN 136:151322  
 TI Efficient syntheses of new **heteroarotinoids** through functional pyridylzinc reagents and palladium-catalyzed cross-coupling reactions  
 AU Alami, Mouad; Peyrat, Jean-Francois; Belachmi, Larbi; Brion, Jean-Daniel  
 CS Laboratoire de Chimie Therapeutique, associe au CNRS (BioCIS), Universite

Paris-Sud, Faculte de Pharmacie, Chatenay-Malabry, 92296, Fr.  
 SO European Journal of Organic Chemistry (2001), (22), 4207-4212  
 CODEN: EJOCFK; ISSN: 1434-193X  
 PB Wiley-VCH Verlag GmbH  
 DT Journal  
 LA English  
 OS CASREACT 136:151322  
 GI



AB A convergent synthesis of **heteroarotinoids** bearing chromene rings in assocn. with pyridyl or ethynylpyridyl moieties, from 6-bromo-2-pyridylzinc chloride is described. This new functional heteroarylzinc reagent, readily accessible from 2,6-dibromopyridine, may undergo a selective palladium-catalyzed carbon-carbon bond-forming reaction to yield the corresponding 6-substituted-2-bromopyridines. Further manipulation of the remaining bromine atom to give the zinc deriv., and subsequent coupling with Et 4-iodobenzoate under palladium catalysis conditions afforded heteroarotinoid I. Coupling of the 6-substituted-2-bromopyridines or Me nicotinate triflate with appropriate alkynes under Sonogashira conditions give the corresponding **heteroarotinoids**, e.g. II.

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

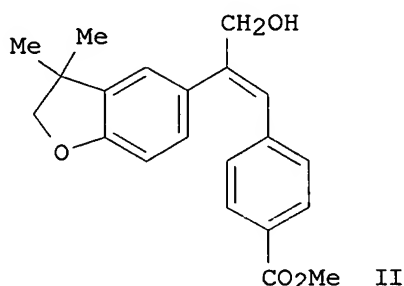
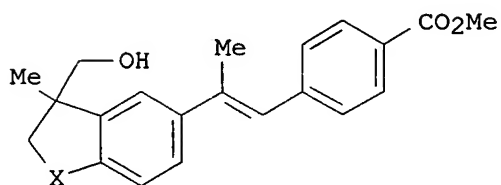
AN 2001:691383 -CAPLUS

DN 136:5846

TI Synthesis of methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-**benzo**[b]thien-5-yl)-1-propenyl]**benzoate**, methyl (E)-4-[2-(2,3-dihydro-3-methyl-3-hydroxymethyl-5-**benzofuranyl**)-1-propenyl] **benzoate**, and methyl (E)-4-[2-(2,3-dihydro-3,3-dimethyl-5-**benzofuranyl**)-3-hydroxy-1-propenyl]**benzoate** as potential metabolites of selected **heteroarotinoids** with fused five-membered rings

AU Gale, Jonathan B.; Klucik, Jozef; Subramanian, Shankar; Berlin, K. Darrell  
 CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078,

USA  
 SO Organic Preparations and Procedures International (2001), 33(5), 487-499  
 CODEN: OPPIAK; ISSN: 0030-4948  
 PB Organic Preparations and Procedures, Inc.  
 DT Journal  
 LA English  
 OS CASREACT 136:5846  
 GI



AB The title compds. I (X = S), I (X= O), and II were prepd. were prepd.  
 stareing from 2-aminothiophenol and 2-nitrophenol.  
 RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic  
 cultures of ovarian carcinoma  
 AN 2001:308164 CAPLUS  
 DN 135:251521  
 TI Effects of retinoids on cancerous phenotype and apoptosis in organotypic  
 cultures of ovarian carcinoma  
 AU Guruswamy, Suresh; Lightfoot, Stan; Gold, Michael A.; Hassan, Raffit;  
 Berlin, K. Darrell; Ivey, R. Todd; Benbrook, Doris M.  
 CS Departments of Obstetrics and Gynecology and Biochemistry and Molecular  
 Biology, University of Oklahoma Health Sciences Center, Oklahoma City, OK,  
 73190, USA  
 SO Journal of the National Cancer Institute (2001), 93(7), 516-525  
 CODEN: JNCIEQ; ISSN: 0027-8874  
 PB Oxford University Press  
 DT Journal  
 LA English  
 AB Background: Retinoic acid analogs, called retinoids, have shown promise in  
 clin. trials in preventing breast and ovarian cancers. Classic retinoids  
 bind to retinoic acid receptors, which regulate cell growth. Some novel  
 retinoids, such as fenretinide, i.e., N-(4-hydroxyphenyl)retinamide  
 (4-HPR), induce apoptosis through retinoic acid receptor-independent  
 mechanisms; however, they appear to do so only at concns. above those  
 achieved in clin. chemoprevention trials. At lower concns. (.1toeq.1  
 .mu.M), 4-HPR acts like classic retinoids, by inducing differentiation

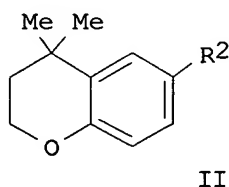
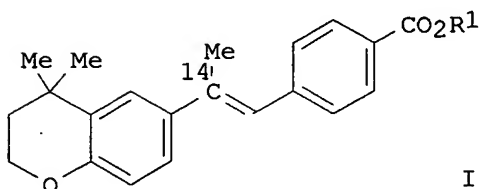
through a receptor-dependent mechanism. Our goal was to compare the effects of novel receptor-independent (apoptotic) retinoids with those of classic growth-inhibitory retinoids at clin. achievable doses on growth, differentiation, and apoptosis in ovarian tissue. Methods: Four receptor-independent (apoptotic) and seven growth-inhibitory retinoids, including synthetic, low-toxicity compds. called **heteroarotinoids**, were administered at concns. of 1 .mu.M to organotypic cultures of ovarian primary and cancer cell lines: OVCAR-3, Caov-3, and SK-OV-3. After fixation, embedding, and sectioning, the growth fraction was quantified by measuring expression of the proliferation marker Ki-67/myb, differentiation was assessed by expression of mucin, and apoptosis was evaluated by the TUNEL assay. Spearman correlation anal. was performed on the data, and all P values were two-sided. Results: All 11 retinoids reversed characteristics assocd. with the cancerous phenotype in all neoplastic cultures. Glandular structures were obsd. consistently in retinoid-treated, but not in untreated, OVCAR-3 and Caov-3 cultures. All retinoids decreased growth fractions, and some increased mucin expression. All receptor-independent retinoids and two receptor-dependent retinoids induced apoptosis, and the induction correlated significantly with increased expression of the mucin MUC1 ( $r = .83$ ;  $P = .03$ ). Retinoids with ester-linking groups did not induce apoptosis but decreased the growth fraction in correlation with MUC1 induction ( $r = -.93$ ;  $P = .02$ ). Conclusions: At clin. achievable concns., all retinoids tested decrease the growth fraction, induce differentiation and apoptosis. Induction of MUC1 expression is implicated in the mechanisms of action.

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2003 ACS  
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]  
AN 1999:803609 CAPLUS  
DN 132:293893  
TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand Interactions of Nitrogen **Heteroarotinoids**. [Erratum to document cited in CA131:310737]  
AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.  
CS Departments Obstetrics Gynecology of Biochem., Molecular Biol. of Otorhinolaryngology and Urology, Univ. Oklahoma Health Sciences Center, Oklahoma City, OK, 73190, USA  
SO Journal of Medicinal Chemistry (2000), 43(2), 303  
CODEN: JMCMAR; ISSN: 0022-2623  
PB American Chemical Society  
DT Journal  
LA English  
AB On page 3606, under Discussion, lines 24 and 25, the ref. to Table 2 is incorrect; Table 1 is the correct ref. The cor. sentence is as follows: "The EC50 value of 6 nM and the 103% efficacy of 2 (Table 1), in comparison to that of 9-c-RA, indicate that 2 may be useful as a pharmaceutical agent for disorders of the skin."

L13 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2003 ACS  
TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C]  
AN 1999:525825 CAPLUS  
DN 131:310738  
TI Optimization and synthesis of (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-**benzopyran**-6-yl)-1-propenyl]**benzoic** acid-11-[14C]  
AU Liu, Shengquan; Berlin, K. Darrell; Simms-Kelley, Melissa D.; Nelson, Eldon C.; Benbrook, Doris M.

CS Department of Chemistry, Oklahoma State University, Stillwater, OK, 74078,  
USA  
SO Journal of Labelled Compounds & Radiopharmaceuticals (1999), 42(8),  
789-796  
CODEN: JLCRD4; ISSN: 0362-4803  
PB John Wiley & Sons Ltd.  
DT Journal  
LA English  
GI



AB **Heteroarotinoids** may be useful in the treatment of skin disorders and a wide variety of cancers. A synthesis of the C-14 labeled heteroarotinoid, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoic acid-11-[14C] (I; R1 = H) is described via a multistep procedure similar to that used to obtain the unlabeled compd. The latter has shown good activity in several assays compared to the std. trans-retinoic acid. Redn. of the carbonyl group in 4,4-dimethylchroman-6-yl Me ketone-(carbonyl-14C) (II; R2 = 13COMe) with LiAlH4 gave alc. II (R2 = 13CHMeOH). Phosphorylation with triphenyl-phosphine hydrobromide in methanol led to the corresponding phosphonium salt II (R2 = 13CHMeP+Ph3Br-). Addn. of n-butyllithium to II (R2 = 13CHMeP+Ph3Br-) in ether at -78.degree.C generated the Wittig reagent in situ and to this was added Et 4-formylbenzoate. Workup and chromatog. afforded E-ester I (R1 = Me) and the Z-ester which were both hydrolyzed to labeled I. Labeled I was identical to the unlabeled isotopomer in terms of spectral data and m.p. The specific activity of I was detd. to be 57.2 .mu.Ci/mg.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI ~~Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand~~  
Interactions of Nitrogen **Heteroarotinoids**

AN 1999:521109 CAPLUS

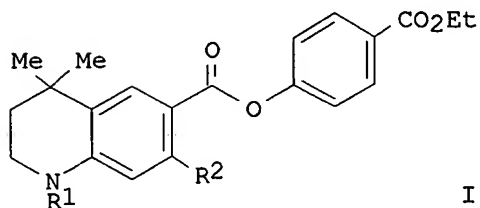
DN 131:310737

TI Synthesis, Structure-Activity Relationships, and RAR.gamma.-Ligand  
Interactions of Nitrogen **Heteroarotinoids**

AU Dhar, Arindam; Liu, Shengquan; Klucik, Jozef; Berlin, K. Darrell; Madler, Matora M.; Lu, Shennan; Ivey, R. Todd; Zacheis, David; Brown, Chad W.; Nelson, E. C.; Birckbichler, Paul J.; Benbrook, Doris M.

CS Departments of Obstetrics Gynecology of Biochemistry Molecular Biology of Otorhinolaryngology and of Urology, University of Oklahoma Health Sciences

Center, Oklahoma City, OK, 73190, USA  
 SO Journal of Medicinal Chemistry (1999), 42(18), 3602-3614  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 GI



AB Three **heteroarotinoids** contg. a nitrogen atom in the first ring and a C-O linking group between the two aryl rings were synthesized and evaluated for RAR and RXR retinoid receptor transactivation, tumor cell growth inhibition, and transglutaminase (TGase) induction. Et 4-(N,4,4-trimethyl-1,2,3,4-tetrahydroquinolinyl)**benzoate** (I; R1 = Me, R2 = H) contained an N-CH3 group and activated all retinoid receptors except for RAR.gamma.. Increasing the hydrophobicity around the rings with analogs Et 4-(N,4,4,7-tetramethyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)**benzoate** (I; R1 = R2 = Me) and Et 4-(4,4-dimethyl-N-isopropyl-1,2,3,4-tetrahydroquinolin-6-oyloxy)**benzoate** (I; R1 = CHMe2, R2 = H) increased the potency and specificity for RAR.alpha., RAR.beta., and RXR.alpha., compared to I (R1 = Me, R2 = H), but had little effect on RXR.beta. and RXR.gamma. activation. Although I (R1 = Me, CHMe2, R2 = H) were unable to activate RAR.gamma., I (R1 = R2 = Me) did activate this receptor with efficacy and high potency equal to that of 9-cis-retinoic acid (II). All three **heteroarotinoids** exhibited 5-8-fold greater specificities for RAR.beta. over RAR.alpha.. In addn., esters I inhibited the growth of two cell lines each derived from cervix, vulvar, ovarian, and head/neck tumors with similar efficiencies to that of II through a mechanism independent of apoptosis. The vulvar cell lines were the most sensitive, and the ovarian lines were the least sensitive. Ester was similar to I (R1 = Me, CHMe2; R2 = H) except that I (R1 = R2 = Me) was a much more potent growth inhibitor of the two vulvar cell lines, which is consistent with strong RAR.gamma. activation by I (R1 = R2 = Me) [but not by I (R1 = Me, CHMe2; R2 = H)] and the high levels of RAR.gamma. expression in skin. All three **heteroarotinoids** induced prodn. of TGase, a marker of retinoid activity in human erythroleukemic cells. Esters I (R1 = R2 = Me; R1 = CHMe2, R2 = H) were the more potent TGase activators than I (R1 = Me, R2 = H), in agreement with the stronger activation of the RAR receptors by I (R1 = R2 = Me; R1 = CHMe2, R2 = H). The biol. activities of these agents, and the RAR.gamma. potency of I (R1 = R2 = Me) in particular, demonstrate the promise of these compds. as pharmaceuticals for cancer and skin disorders.

RE.GNT 40-- THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI synthesis, receptor specificity and TGase activity of  
**heteroarotinoids**-anticancer agents  
 AN 1998:147324 CAPLUS  
 DN 128:204998  
 TI synthesis, receptor specificity and TGase activity of  
**heteroarotinoids**-anticancer agents  
 IN Berlin, Kenneth Darrel; Subramanian, Shanker; Nelson, Eldon Carl; Madler,

Matora May; Patterson, Manford Kenneth, Jr.; Birckbichler, Paul Joseph;  
Benbrook, Doris Mangiaracina

PA Board of Regents for Oklahoma State University, USA

SO PCT Int. Appl., 93 pp.

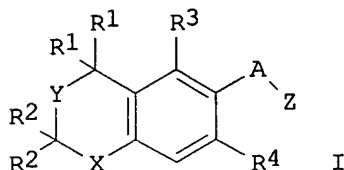
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

|    | PATENT NO.                                                             | KIND | DATE     | APPLICATION NO.  | DATE     |
|----|------------------------------------------------------------------------|------|----------|------------------|----------|
| PI | WO 9807716                                                             | A2   | 19980226 | WO 1997-US14720  | 19970821 |
|    | W: AU, CA, CN, JP                                                      |      |          |                  |          |
|    | RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE |      |          | US 1996-24521P P | 19960823 |
|    | AU 9740805                                                             | A1   | 19980306 | AU 1997-40805    | 19970821 |
|    |                                                                        |      |          | US 1996-24521P P | 19960823 |
|    |                                                                        |      |          | WO 1997-US14720W | 19970821 |
| OS | MARPAT 128:204998                                                      |      |          |                  |          |
| GI |                                                                        |      |          |                  |          |



AB Synthesis of heteroarotinoid structures (I) [R1 = H, Me; R2 = H, Me; R3 = H, Me; R4 = H, Me, OMe; A = CO2, O2C, CONH, CONOH, CONOMe, NHCO, C(Me)=CH, COCH=CH; X = O, S, SO, SO2, NMe, NEt, NPr, NCHMe2, CMe2; Y = CH2, O, S; Z = C6H4-4-CO2R, C6H4-3-CO2R, C6H3-3-Me-4-CO2R, C6H3-2-Me-4-CO2R, CH=CHCH=CHCO2R, CH=CHC(Me)=CHCO2R; R = H, Me, Et, Pr, CHMe2] partially related to trans-retinoic acid through the basic, fused-ring framework and having receptor specificity as well as activity in stimulating formation of the enzyme transglutaminase as a marker for anticancer activity is reported. Thus, I (R1=R2 = Me, R3=R4 = H, Y = CH2, X = S, A = NHCO, Z = C6H3-2-Me-4-CO2R, R = H) (II) is prepd. in 68% yield by NaOH hydrolysis of the corresponding ester in ethanol formed by the condensation of 6-amino-2,3-dihydro-2,2,4,4-tetramethyl-2H-1-benzothiopyran with monomethyl terephthaloyl chloride. II shows an R value of 0.76 as compared to trans-retinoic acid in TGase assay.

L13 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AN 1997:638457 CAPLUS

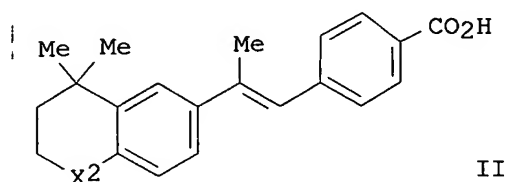
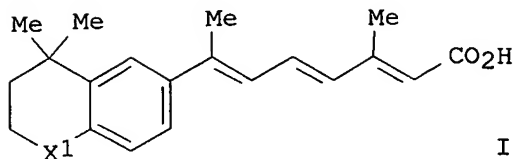
DN 127:307506

TI Biologically Active **Heteroarotinoids** Exhibiting Anticancer Activity and Decreased Toxicity

AU Benbrook, Doris M.; Madler, Matora M.; Spruce, Lyle W.; Birckbichler, Paul J.; Nelson, Eldon C.; Subramanian, Shankar; Weerasekare, G. Mahika; Gale, Jonathan B.; Patterson, Manford K., Jr.; Wang, Binghe; Wang, Wei; Lu, Shennan; Rowland, Tami C.; DiSivestro, Paul; Lindamood, Charles; Hill, Donald L.; Berlin, K. Darrell

CS Departments of Obstetrics Gynecology Urology and Medicinal Chemistry and Pharmaceuticals, University of Oklahoma Health Sciences Center, Oklahoma City, OK, 73L90, USA

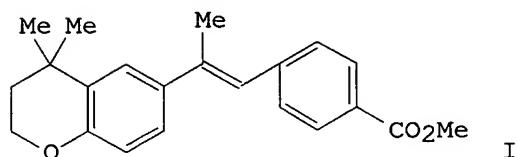
SO Journal of Medicinal Chemistry (1997), 40(22), 3567-3583



AB A series of retinoids, contg. heteroatoms in a cyclic ring and called **heteroarotinoids**, were synthesized, and their biol. activity was evaluated using tissue culture lines that have measurable responses to trans-retinoic acid (t-RA). Transglutaminase (TGase) was assessed in the human erythroleukemia cell line (GMO6141A) as an indicator of differentiation and apoptosis. Proliferation was evaluated in a human cervical cell line, CC-1, which exhibits dose-dependent alterations in growth rate in response to treatment with trans-retinoic acid. Activation of nuclear retinoic acid receptors was detd. in a reporter cell line established from CC-1. The reporter line, called CC-B, contains a reporter gene controlled by a retinoic acid responsive element (RARE) and a thymidine kinase (tk) promoter. Treatment of the CC-B line with the **heteroarotinoids** resulted in a dose-responsive and retinoid-dependent regulation of reporter gene expression. The **heteroarotinoids** exhibited activity in all assays and correlated in a statistically significant manner between assays. RARE transactivation activity in CC-B cells correlated with induction of TGase in GMO6141A ( $R = 0.96$ ) and with a decrease in the growth rate of CC-1 cells ( $R = -0.90$ ). The ability of the selected **heteroarotinoids** to induce differentiation, inhibit proliferation, and activate nuclear receptors demonstrates the chemotherapeutic potential of these agents. In view of the biol. activity cited, an in vivo toxicity study was conducted on male B6D2F1 mice with three **heteroarotinoids**, namely (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylthiochroman-6-yl)-2,4,6-heptatrienoic acid (I;  $X1 = S$ ), (2E,4E,6E)-3,7-dimethyl-7-(1,2,3,4-tetrahydro-4,4-dimethylchroman-6-yl)-2,4,6-heptatrienoic acid (I;  $X1 = O$ ), and (E)-p-[2-(4,4-dimethylchroman-6-yl)propenyl]benzoic acid (II;  $X2 = O$ ). The mice were used with gavage of **heteroarotinoids** in corn oil [0.1, 0.2, 0.4, or 0.8 mg/kg] and with 0.01 or 0.05 mg/kg of (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]benzoic acid [TTNPB (II;  $X2 = CMe_2$ )] as ref. controls. The target organs affected in the mice by the three **heteroarotinoids** were those typically assocd. with trans-retinoic acid (III) toxicity. The max. tolerated dose (MTD) of 13 was 9.4 mg/kg/day, which was equal in toxicity to that of III and 1000-fold less toxic than TTNPB. The MTDs of I were 34 and 32 mg/kg/day,

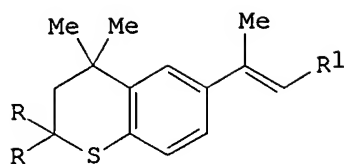
resp., which is 3-fold less toxic than III and 3000-fold less toxic than TTNPB. The 3000-fold reduced toxicity, compared with only a 27% redn. biol. activity of I with respect to that of TTNPB, obsd. in our assays indicates a good therapeutic ratio of these **heteroarotinoids** over the parent compd. The biol. activity and reduced toxicity of these **heteroarotinoids** demonstrate the potential efficacy as anticancer agents.

L13 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI **Heteroarotinoids:** crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate**  
 AN 1992:6745 CAPLUS  
 DN 116:6745  
 TI **Heteroarotinoids:** crystal and molecular structure analysis of the methyl (Z)- and methyl (E)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate**  
 AU Welsh, William J.; Cody, Vivian; Suwinski, Kinga; Berlin, K. Darrell; Rajadhyaksha, Shirish N.; Subramanian, Shankar; Verma, A. K.  
 CS Dep. Chem., Univ. Missouri, St. Louis, MO, 63121, USA  
 SO Structural Chemistry (1991), 2(5), 515-22  
 CODEN: STCHES; ISSN: 1040-0400  
 DT Journal  
 LA English  
 GI



AB Crystal structures and MM2P mol. mechanics force-field and AM1 MO calcns. were performed on Me (E)- and Me (Z)-4-[2-(4,4-dimethylchroman-6-yl)-1-propenyl] **benzoate** (I) and confirmed that the calcd. mol. structures are in good agreement with the obsd. crystallog. conformations which show that both isomers have a twist-sofa oxo ring conformation and nearly perpendicular arom. ring systems, resp. Full relaxation MM2P conformational energy profiles for the rotation about the propenyl bridge indicate that the max. energy barrier is less than 3.5 kcal/mol.

L13 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Novel **heteroarotinoids:** synthesis and biological activity  
 AN 1991:114595 CAPLUS  
 DN 114:114595  
 TI Novel **heteroarotinoids:** synthesis and biological activity  
 AU Spruce, Lyle W.; Gale, Jonathan B.; Berlin, K. Darrell; Verma, A. K.; Breitman, Theodore R.; Ji, Xinhua; Van der Helm, Dick  
 CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA  
 SO Journal of Medicinal Chemistry (1991), 34(1), 430-9  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 OS CASREACT 114:114595  
 GI



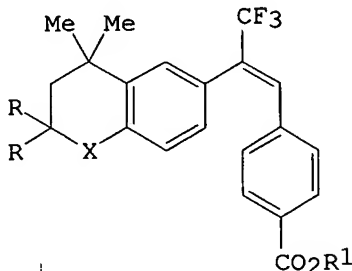
I, R=Me, R<sup>1</sup>=C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>Me-4

II, R=Me, R<sup>1</sup>=C<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>H-4

IV, R=H, R<sup>1</sup>=E, E-CH=CHCMe=CO<sub>2</sub>H

V, R=Me, R<sup>1</sup>=E, Z-CH=CHCMe=CO<sub>2</sub>H

VI, R=H, R<sup>1</sup>=E-CH=CH ...CO<sub>2</sub>H



VII, R=R<sup>1</sup>=Me, X=S

VIII, R=Me, R<sup>1</sup>=H, X=S

IX, R=H, R<sup>1</sup>=Me, X=S

X, R=R<sup>1</sup>=H, X=S

XI, R=H, R<sup>1</sup>=Me, X=O

XII, R=R<sup>1</sup>=H, X=O

AB Thirteen **heteroarotinoids** were synthesized. The key step in each prepn. was the condensation of the appropriate chroman-, thiochroman-, or **benzothieryl**-substituted phosphorus ylide, obtained from the independent synthesis of the corresponding phosphonium salts, with selected polyene-substituted aldehyde esters. Screening of the compds. was with one of two assays. One assay measured the ability of a retinoid to inhibit the phorbol ester induced increase of mouse epidermal ornithine decarboxylase (ODC) activity. The other assay measured retinoid-induced differentiation of the human myeloid leukemia cell line HL-60. In the ODC assay, all thirteen compds. were screened. The most active **heteroarotinoids** were ester I and the acid II. Both of these retinoids had ID<sub>50</sub> values (dose required for half-maximal inhibition of phorbol ester induced ODC activity) of about 0.3 nmol. In comparison, the ID<sub>50</sub> value for trans-retinoic acid III was 0.12 nmol while the ID<sub>50</sub> values for acids IV and V were about 3.5 nmol. **Heteroarotinoids** VI and VII-XII had ID<sub>50</sub> values of 35 nmol or greater. With a thiochroman unit, the most active acids in decreasing order of activity in the ODC assay were II > V > VI. Thus, simple replacement of the terminal propenyl system [C(16,17,18)] in IV with a cyclopropyl group produced acid VI with markedly reduced activity. With a **benzoic** acid group as part of the structure attached to the thiochroman unit, the ODC activity was enhanced as shown in I and II. The combination of the 2,2,4,4-tetramethylthiochroman group and the **benzoic** acid (or ester) terminal group seemed to enhance the biol. action which resembles that found with (E)-4-[2-(5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)-1-propenyl]**benzoic** acid, a well-known model system. Replacing the protons with fluorine in the C(12) Me group in the side chain and altering the orientation of the aryl groups around the double bond from anti to syn lowered ODC activity in both the thiochroman- and chroman-contg. systems. Esters VII and IX and acid VIII were essentially inactive while acid X exhibited a high ID<sub>50</sub> in the ODC assay. In the chroman family, both ester XI and acid XII had unfavorable ID<sub>50</sub> values. Since acid VIII differs only slightly from acid X [the latter is devoid of the geminal di-Me group at C(2)] and acid X differs only slightly from acid XII, possibly the nature of the heteroatom and the stereochem. at the .alpha. position may play important roles in regulating activity, but more examples are required to establish a trend. Changing the ring size from a fused six-six system to a five-six system led to ester Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoate** (XIII) and acid (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]**benzoic** acid (XIV),

resp. In sep. expts. from those with of I-XII and known compds both XIII and XIV exhibited similar inhibition of ODC activity to that of III at the 34 nmol level. The ID50 values of XIV and XIV were, however, 10 and 200 times greater than that of III resp. In view of the toxicity of III, ester XIII may hold promise in chemotherapy. Of eight **heteroarotinoids** examd. in the HL-60 assay system, only acid IV displayed modest activity. This acid had an ED50 value (dose required for half-maximal effect) of 500 nM. In comparison, the ED50 for III was 50 nM. All of the other **heteroarotinoids** had ED50 values which were greater than 1000 nM.

L13 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI **Heteroarotinoids:** analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples

AN 1990:424286 CAPLUS

DN 113:24286

TI **Heteroarotinoids:** analytical criteria for the rapid identification of E and Z isomers of these novel retinoids via NMR, UV, and x-ray analyses of selected examples

AU Gale, Jonathan B.; Rajadhyaksha, Shirish N.; Spruce, Lyle W.; Berlin, K. Darrell; Ji, Xinhua; Slagle, Andrew; Van der Helm, Dick

CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA

SO Journal of Organic Chemistry (1990), 55(13), 3984-91  
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

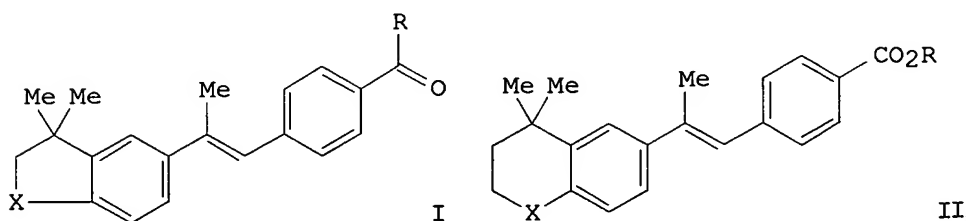
OS CASREACT 113:24286

AB A series of derivs. of E and Z isomers of 4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoic acid and 4-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-1-propenyl]benzoic acid and sulfur-contg. counterparts were examd. in terms of <sup>1</sup>H, <sup>13</sup>C, and UV analyses for the purpose of establishing which parameters are diagnostic for identifying E and Z isomers in this family of **heteroarotinoids**. In addn., x-ray diffraction analyses for Me (E)-[2-(2,3-dihydro-3,3-dimethyl-5-benzofuranyl)-1-propenyl]benzoate (I), Me (E)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]benzoate (II), and Me (Z)-4-[2-(2,3-dihydro-3,3-dimethylbenzo[b]thien-5-yl)-1-propenyl]benzoate (III) were performed to confirm the arrangement around the central double bond in the solid state in these rare examples contg. a fused, five-six-membered ring system. The proton NMR analyses of solns. of the E vs. the Z isomers, particularly the enhanced shielding of the vinylic proton and protons at "ortho" positions on the aryl groups attached to the double bond, provide markers to identify the Z isomers in these **heteroarotinoids**. In the <sup>13</sup>C spectra, the Me C attached to the double bond was usually about 10 ppm downfield in the Z isomer compared to the counterpart in the E isomer. These data suggest that in soln. the two aryl rings in the Z isomers, (and possibly the E isomers, are turned out of the plane of the double bond, and, due to the closer proximity of the rings, induced shielding of nearby protons occurs to a greater extent in the Z isomers, compared to the E isomers. This evaluation is supported by UV spectral data which show max. in two ranges, namely at 210-270 and 280-350 nm. The "conjugation band" at the longer wavelength is always more intense, relative to the band at the shorter wavelength, in the E isomers. This implies improved overlap of p orbitals in the double bond with those in the aryl rings in the E isomers. In contrast, the band at shorter wavelength is more intense than the band at long wavelength in the Z isomers. These two features are clearly distinguishing for the two isomeric forms in soln. and relate to some degree to the stilbene isomerism. Characterization of I, II, and III via x-ray diffraction anal. of single crystals confirmed that the rings in both isomeric alkenes lack coplanarity with the central double bond in the solid state. The deviation from overall planarity is greatest for the Z

isomers with the internal torsional angle being 10.1.degree. in III rather than the "ideal" value of 0.degree.. Moreover, the aryl rings are not far from being nearly perpendicular to each other in III. Mol. mechanics calcs., using the MMP2 program, indicate that the deviation from planarity is less than that found from x-ray anal. on solid III. These data provide a foundation for rapid identification of certain groups of **heteroarotinoids**. A comparison of crystal data of I and II with that of trans-retinoic acid was also made. The least-squares "fit" is quite satisfactory in spite of differences in conformational angles, and an RMS value of 0.90 .ANG. is calcd.

L13 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI Heteroarotinoid compounds as anticancer agents  
 AN 1989:573986 CAPLUS  
 DN 111:173986  
 TI Heteroarotinoid compounds as anticancer agents  
 IN Berlin, Kenneth D.; Holt, Elizabeth M.; Ford, Warren T.; Thompson, Mark D.  
 PA Oklahoma State University, USA  
 SO U.S., 18 pp. Cont.-in-part of U.S. Ser. No. 598,482, abandoned.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

|    | PATENT NO.                             | KIND | DATE     | APPLICATION NO. | DATE     |
|----|----------------------------------------|------|----------|-----------------|----------|
| PI | US 4826984                             | A    | 19890502 | US 1987-9083    | 19870127 |
|    |                                        |      |          | US 1984-598482  | 19840409 |
| OS | CASREACT 111:173986; MARPAT 111:173986 |      |          |                 |          |
| GI |                                        |      |          |                 |          |

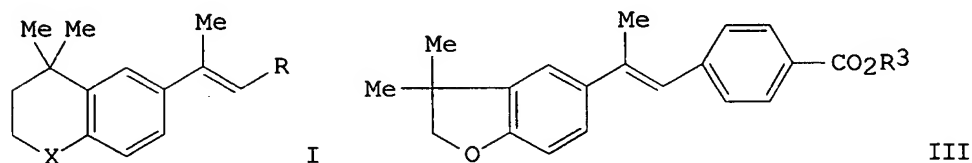


AB **Heteroarotinoids**, e.g., I (R = H, OH, OMe, OEt, etc.; X = S, SO, O), II (R = H, Me, Et; X = O, S, SO), etc., were prepd. as anticancer agents. Treatment of [1-(3,4-dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)ethyl]triphenylphosphonium bromide (prepn. given) with BuLi, followed by reaction with Et 4-formylbenzoate, gave, after workup, Et (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzothiopyran-6-yl)-1-propenyl]benzoate. In the HL-60 cell differentiation assay, (E)-4-[2-(3,4-dihydro-4,4-dimethyl-2H-1-benzopyran-6-yl)-1-propenyl]benzoate exhibited an ED50 of > 3 .mu.M, vs. an ED50 of 200 nM for tetrahydrotetramethylnaphthalenylpropenylbenzoic acid.

L13 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2003 ACS  
 TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells  
 AN 1987:576259 CAPLUS  
 DN 107:176259  
 TI **Heteroarotinoids**. Synthesis, characterization, and biological activity in terms of an assessment of these systems to inhibit the

induction of ornithine decarboxylase activity and to induce terminal differentiation of HL-60 cells

AU Spruce, Lyle W.; Rajadhyaksha, Shirish N.; Berlin, K. Darrell; Gale, Jonathan B.; Miranda, Edgar T.; Ford, Warren T.; Blossey, Erich C.; Verma, A. K.; Hossain, M. B.; et al.  
CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA  
SO Journal of Medicinal Chemistry (1987), 30(8), 1474-82  
CODEN: JMCMAR; ISSN: 0022-2623  
DT Journal  
LA English  
OS CASREACT 107:176259  
GI



AB The heteroarotenoids I (X = S, R = CH:CHCMe:CHCO<sub>2</sub>R<sub>1</sub>, R<sub>1</sub> = H, Et, 2-phthalimidoethyl) were prepd. from 6-acetyl-4,4-dimethylthiochroman. I (X = O, R = CH:CHCMe:CHCO<sub>2</sub>H) was similarly obtained from 6-acetyl-4,4-dimethylchroman (II). I (X = O, R = 4-R<sub>2</sub>C<sub>6</sub>H<sub>4</sub>, R<sub>2</sub> = CO<sub>2</sub>Me, CH<sub>2</sub>OH, cyano, CHO) were also obtained from II. **Benzofurans** III (R<sub>3</sub> = Me, H) were prepd. from 4-MeOC<sub>6</sub>H<sub>4</sub>Br and CH<sub>2</sub>:CMeCH<sub>2</sub>Cl. I (R = CH:CHCMe:CHCO<sub>2</sub>R<sub>1</sub>) showed high inhibition of ornithine decarboxylase, whereas I (R = 4-R<sub>2</sub>C<sub>6</sub>H<sub>4</sub>) and III were somewhat less active. In the HL-60 cell differentiation test I and III were substantially less active than trans-retinoic acid.

L13 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2003 ACS

TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**.

AN 1985:24869 CAPLUS

DN 102:24869

TI Synthesis and characterization of selected **heteroarotinoids**. Pharmacological activity as assessed in vitamin A deficient hamster tracheal organ cultures. Single-crystal x-ray diffraction analysis of 4,4-dimethylthiochroman-6-yl methyl ketone 1,1-dioxide and ethyl (E)-p-[2-(4,4-dimethylthiochroman-6-yl)propenyl]**benzoate**.

AU Waugh, Kristy M.; Berlin, K. Darrell; Ford, Warren T.; Holt, Elizabeth M.; Carrol, John P.; Schomber, Paul R.; Thompson, M. Daniel; Schiff, Leonard J.

CS Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA

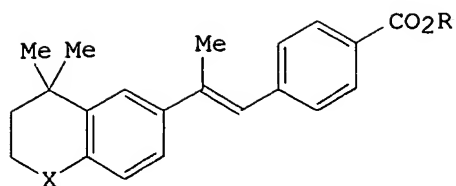
SO Journal of Medicinal Chemistry (1985), 28(1), 116-24

CODEN: JMCMAR; ISSN: 0022-2623

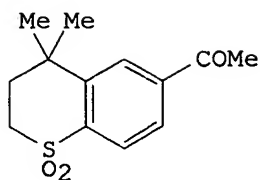
DT Journal

LA English

GI



I



III

AB **Heteroarotinoids** I [X, R = S, Et (II); O, Et; S(O), Et; O, H] and the dioxide III were prepd. and evaluated for their vitamin A activity. X-ray anal. data for II and III are given.

=> logoff hold

|                                            |            |         |
|--------------------------------------------|------------|---------|
| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |
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|                                            | ENTRY      | SESSION |
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=> file reg

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| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 77.67      | 77.88   |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
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DICTIONARY FILE UPDATES: 4 JUL 2003 HIGHEST RN 542812-68-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading 10075845 clm 9.str

L15 STRUCTURE UPLOADED

=> d l15

L15 HAS NO ANSWERS

L15 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search l15 sss sam

SAMPLE SEARCH INITIATED 13:45:16 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 135 TO ITERATE

100.0% PROCESSED 135 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2003 TO 3397

PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15

=> search l15 sss full

FULL SEARCH INITIATED 13:45:25 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3132 TO ITERATE

100.0% PROCESSED 3132 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

L17 0 SEA SSS FUL L15

=>

Uploading 10075845 clm 9.str

L18 STRUCTURE UPLOADED

=> d l18

L18 HAS NO ANSWERS

L18 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> search l18 sss sam  
SAMPLE SEARCH INITIATED 13:46:55 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 135 TO ITERATE

100.0% PROCESSED 135 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2003 TO 3397  
PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L18

=> search l18 sss full  
FULL SEARCH INITIATED 13:47:03 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3132 TO ITERATE

100.0% PROCESSED 3132 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L20 0 SEA SSS FUL L18

|                                            |            |         |
|--------------------------------------------|------------|---------|
| => logoff hold                             |            |         |
| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 297.10     | 374.98  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |
| CA SUBSCRIBER PRICE                        | 0.00       | -11.72  |

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|                                            |            |         |
|--------------------------------------------|------------|---------|
| COST IN U.S. DOLLARS                       | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |
| FULL ESTIMATED COST                        | 297.10     | 374.98  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
|                                            | ENTRY      | SESSION |